

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 20

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 7-20 8-9 8-13 9-10 11-12 11-20 12-13  
12-14 13-17 14-15 15-16 16-17

exact/norm bonds :

4-7 5-10 7-8 7-20 8-9 8-13 9-10 11-12 11-20

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-14 13-17 14-15 15-16 16-17

G1:O,S,C

G2:O,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 20:Atom

10/307,735

=> d his

(FILE 'HOME' ENTERED AT 16:57:45 ON 23 MAR 2005)

FILE 'REGISTRY' ENTERED AT 16:57:50 ON 23 MAR 2005

L1 STRUCTURE UPLOADED  
L2 2 S L1  
L3 286 S L1 SSS FUL

FILE 'CAPLUS' ENTERED AT 17:02:00 ON 23 MAR 2005

L4 109 S L3  
L5 ANALYZE L4 1- RN HIT : 263 TERMS

FILE 'REGISTRY' ENTERED AT 17:02:26 ON 23 MAR 2005

L6 3 S 191-28-6/RN OR 3779-11-1/RN OR 13225-81-5/RN  
L7 STRUCTURE UPLOADED  
L8 5 S L7  
L9 568 S L7 SSS FUL

FILE 'CAPLUS' ENTERED AT 17:07:30 ON 23 MAR 2005

L10 186 S L9

FILE 'REGISTRY' ENTERED AT 17:07:42 ON 23 MAR 2005

FILE 'CAPLUS' ENTERED AT 17:08:14 ON 23 MAR 2005  
S C16 H8 O4/MF

FILE 'REGISTRY' ENTERED AT 17:08:33 ON 23 MAR 2005

FILE 'CAPLUS' ENTERED AT 17:08:34 ON 23 MAR 2005

FILE 'REGISTRY' ENTERED AT 17:08:46 ON 23 MAR 2005

L11 88 S C16 H8 O4/MF  
L12 1 S L11 AND L6  
L13 565 S L9 NOT L6

FILE 'CAPLUS' ENTERED AT 17:09:31 ON 23 MAR 2005

L14 144 S L13  
L15 ANALYZE L14 1- RN HIT : 484 TERMS

FILE 'REGISTRY' ENTERED AT 17:11:50 ON 23 MAR 2005

L16 164625 S 6-6-6-6/SZ  
L17 12949 S 6-6-6-7/SZ  
L18 1215 S 6-6-6-8/SZ  
L19 178780 S L16 OR L17 OR L18  
L20 294 S L9 AND L19  
L21 274 S L9 NOT L20

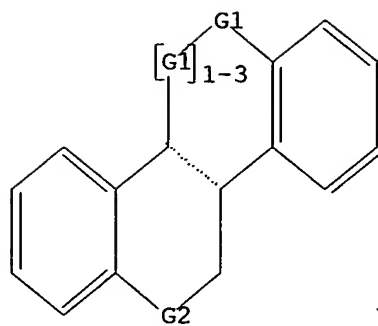
FILE 'CAPLUS' ENTERED AT 17:23:55 ON 23 MAR 2005

L22 58 S L20

=> d 17

L7 HAS NO ANSWERS  
L7 STR

10/307,735



G1 O, S, C

G2 O, S

Structure attributes must be viewed using STN Express query preparation.

=> d ibib abs hitstr 1-58

oppl 122 ANSWER 1 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

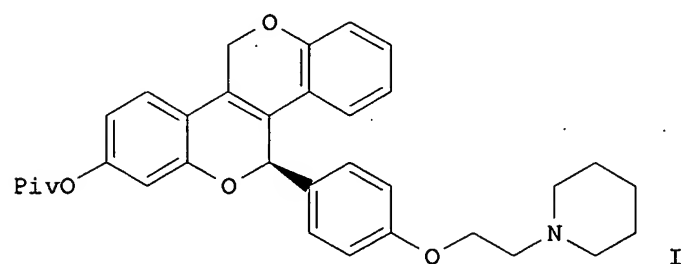
ACCESSION NUMBER: 2004:1127099 CAPLUS  
 DOCUMENT NUMBER: 142:56279  
 TITLE: Preparation of tetracyclic heterocycles as selective estrogen receptor modulators (SERMs).  
 INVENTOR(S): Kanojia, Ramesh M.; Jain, Nareshkumar F.; Ng, Raymond; Sui, Zhihua; Xu, Jiayi  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 110 pp., Cont.-in-part of U.S. Ser. No. 307,735.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004259915	A1	20041223	US 2003-719875	20031121
US 2003216463	A1	20031120	US 2002-307735	20021202
WO 2004050660	A1	20040617	WO 2003-US37419	20031121

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2001-341957P P 20011219  
 US 2002-307735 A2 20021202

GI



AB There are 5 claimed compds., e.g., I and over 100 synthetic examples of selective estrogen receptor modulators. Thus, 3-(2-hydroxy-4-methoxyphenyl)-7-hydroxy-4-methylchromen-2-one (preparation given), in methanol/acetone was added at room temperature anhydrous potassium carbonate; the solution was stirred 2 h to give 2,8-dihydroxy-1H-chromeno[4,3-c]chromen-5-one. The latter bound to estrogen  $\alpha$  and  $\beta$  receptors at 0.505  $\mu$ M and 0.061  $\mu$ M, resp. I are useful in the treatment and/or prevention of disorders associated with the depletion of estrogen such as hot flashes, vaginal dryness, osteopenia and osteoporosis; hormone sensitive



cancers and hyperplasia of the breast, endometrium, cervix and prostate; endometriosis, uterine fibroids, osteoarthritis and as contraceptive agents, alone or in combination with a progestogen or progestogen antagonist.

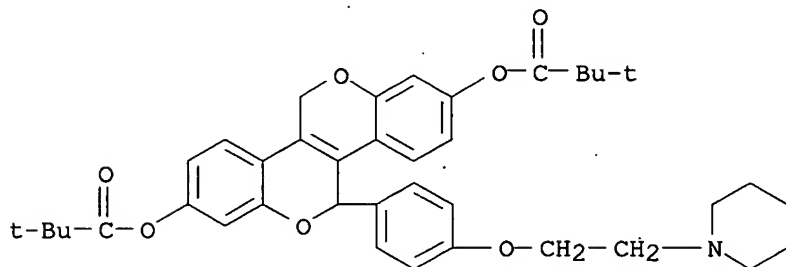
IT 554429-87-7P 554429-88-8P 554429-89-9P  
554429-90-2P 554429-91-3P 554429-92-4P  
554429-93-5P 554429-94-6P 554429-95-7P  
554429-96-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of tetracyclic heterocycles as selective estrogen receptor modulators (SERMs))

RN 554429-87-7 CAPLUS

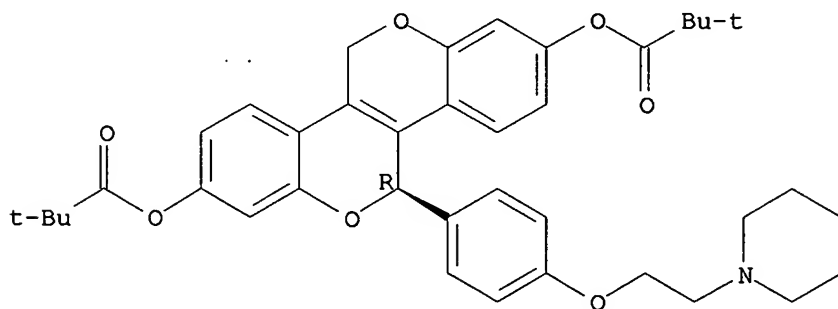
CN Propanoic acid, 2,2-dimethyl-, 5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl ester (9CI) (CA INDEX NAME)



RN 554429-88-8 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, (5R)-5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl ester (9CI) (CA INDEX NAME)

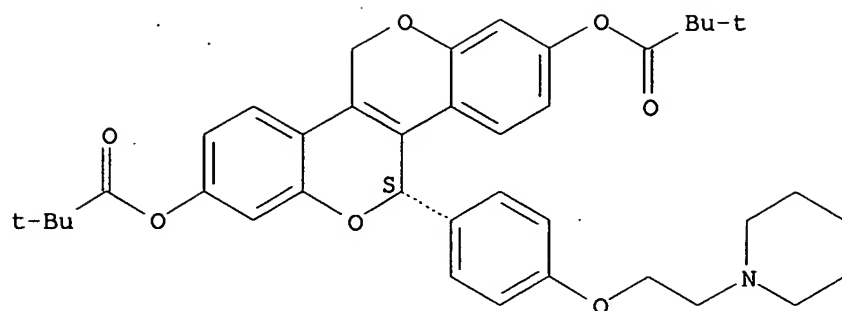
Absolute stereochemistry.



RN 554429-89-9 CAPLUS

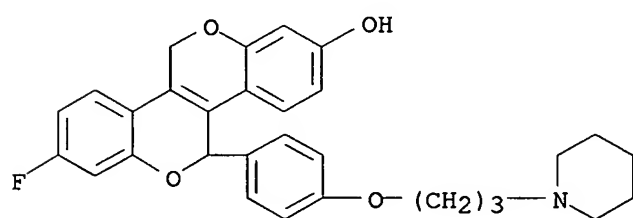
CN Propanoic acid, 2,2-dimethyl-, (5S)-5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



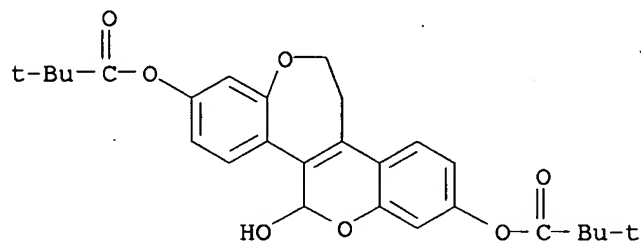
RN 554429-90-2 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2-ol, 8-fluoro-5,11-dihydro-5-[4-[3-(1-piperidinyl)propoxy]phenyl]- (9CI) (CA INDEX NAME)



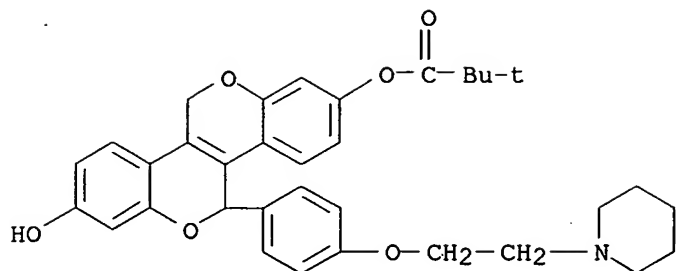
RN 554429-91-3 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 11,12-dihydro-5-hydroxy-5H-[1]benzopyrano[4,3-d][1]benzoxepin-2,8-diyl ester (9CI) (CA INDEX NAME)



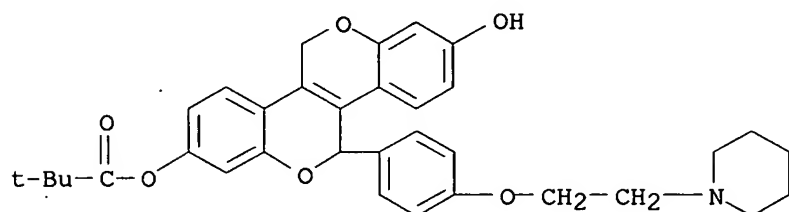
RN 554429-92-4 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 5,11-dihydro-8-hydroxy-5-[4-[3-(1-piperidinyl)propoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2-yl ester (9CI) (CA INDEX NAME)



RN 554429-93-5 CAPLUS

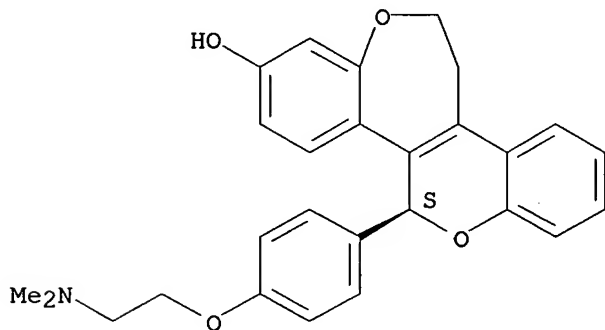
CN Propanoic acid, 2,2-dimethyl-, 5,11-dihydro-8-hydroxy-11-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2-yl ester (9CI) (CA INDEX NAME)



RN 554429-94-6 CAPLUS

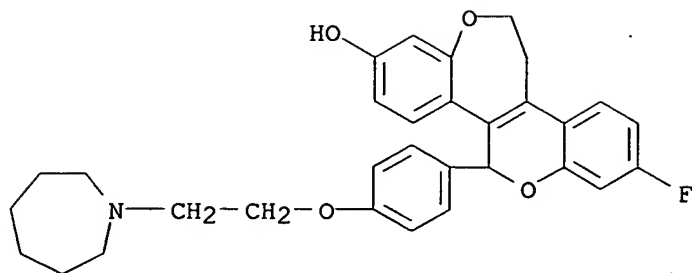
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 5-[4-[2-(dimethylamino)ethoxy]phenyl]-11,12-dihydro-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 554429-95-7 CAPLUS

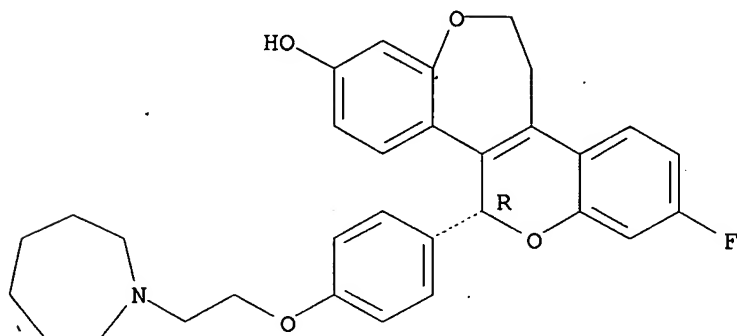
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 8-fluoro-5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro- (9CI) (CA INDEX NAME)



RN 554429-96-8 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 8-fluoro-5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro-, (5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 554429-97-9P 554430-39-6P 554430-43-2P  
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 554430-60-3P 554430-85-2P 554430-86-3P  
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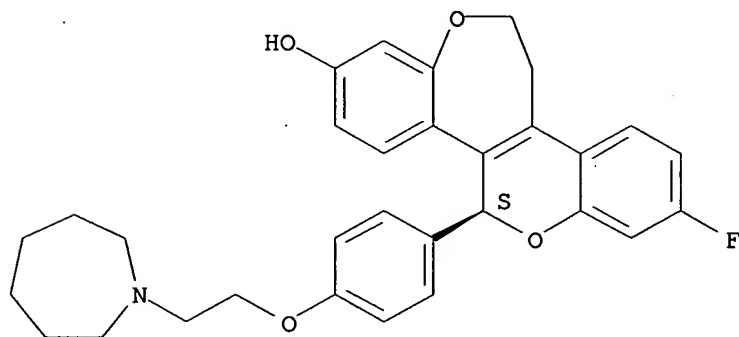
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of tetracyclic heterocycles as selective estrogen receptor modulators (SERMs))

RN 554429-97-9 CAPLUS

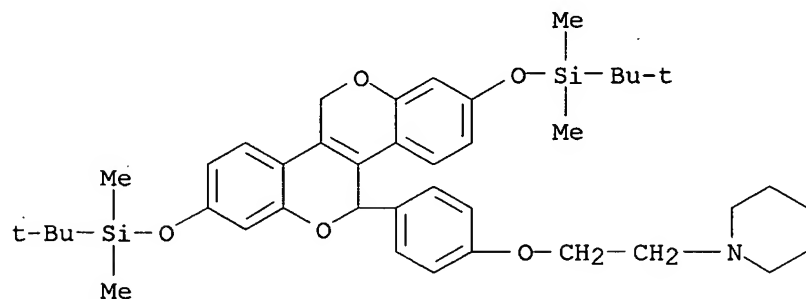
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 8-fluoro-5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 554430-39-6 CAPLUS

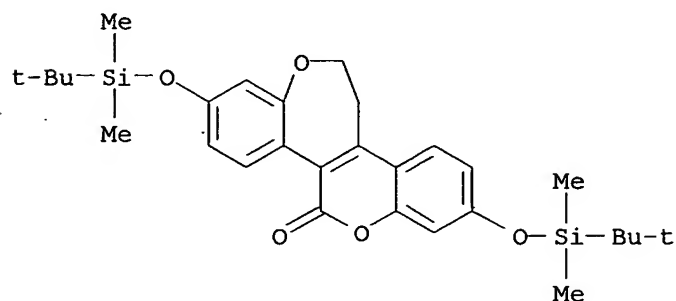
CN Silane, [[5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



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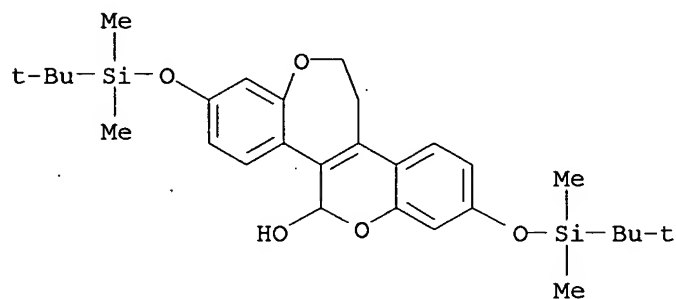
RN 554430-43-2 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro- (9CI) (CA INDEX NAME)



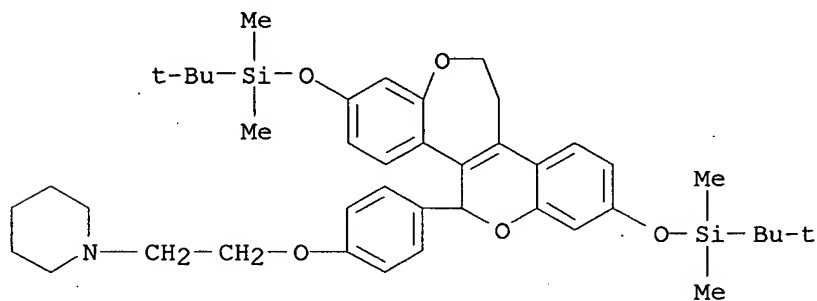
RN 554430-44-3 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-ol, 2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro- (9CI) (CA INDEX NAME)



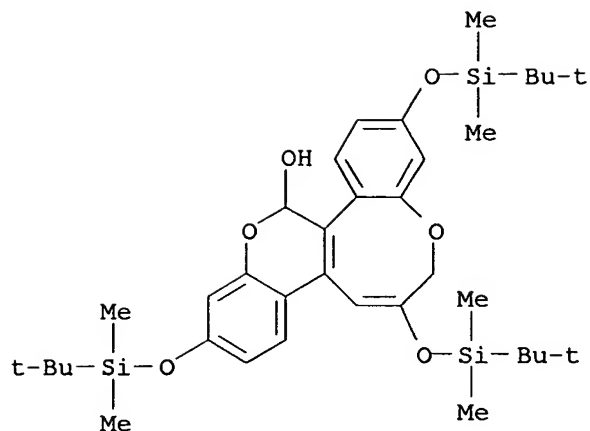
RN 554430-45-4 CAPLUS

CN Piperidine, 1-[2-[4-[2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



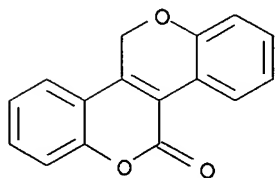
RN 554430-48-7 CAPLUS

CN [1]Benzopyrano[4,3-e][1]benzoxocin-13-ol, 2,6,10-tris[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7,13-dihydro- (9CI) (CA INDEX NAME)

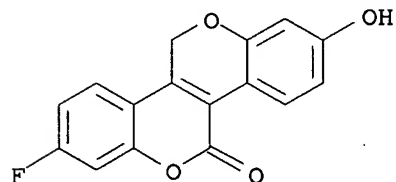


RN 554430-60-3 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5(11H)-one (9CI) (CA INDEX NAME)

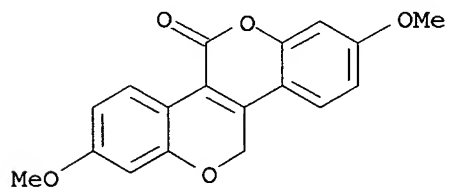


RN 554430-85-2 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5(11H)-one, 8-fluoro-2-hydroxy- (9CI)  
(CA INDEX NAME)

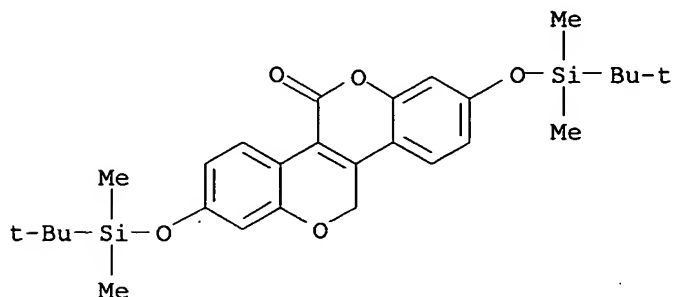
RN 554430-86-3 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5(11H)-one, 2,8-dimethoxy- (9CI) (CA INDEX NAME)



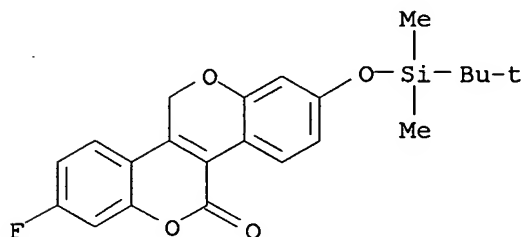
RN 554430-87-4 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5(11H)-one, 2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]- (9CI) (CA INDEX NAME)



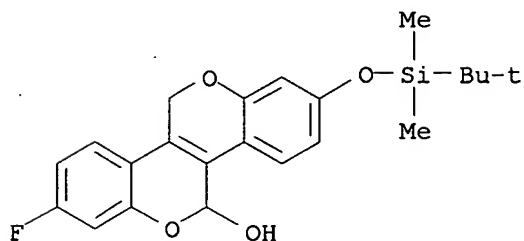
RN 554430-88-5 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5(11H)-one, 2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-fluoro- (9CI) (CA INDEX NAME)



RN 554430-89-6 CAPLUS

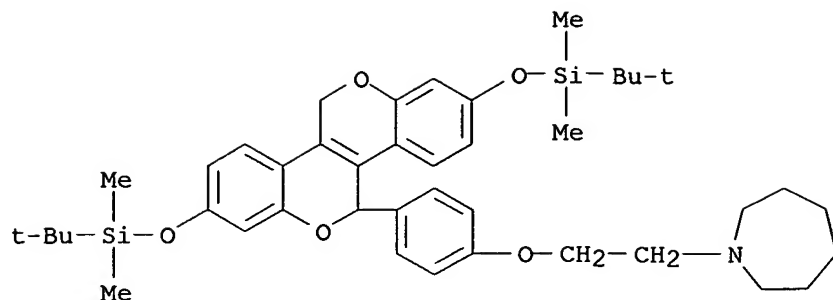
CN [1]Benzopyrano[4,3-c][1]benzopyran-5-ol, 2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-fluoro-5,11-dihydro- (9CI) (CA INDEX NAME)



RN 554430-90-9 CAPLUS

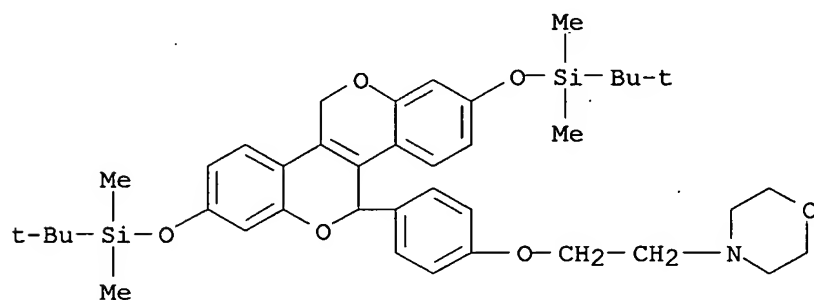
CN 1H-Azepine, 1-[2-[4-[2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]hexahydro- (9CI) (CA INDEX NAME)





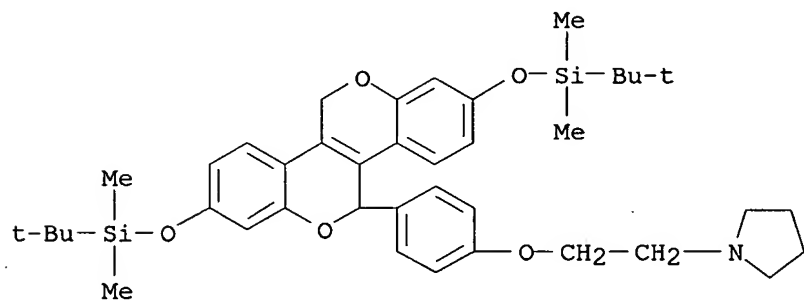
RN 554430-91-0 CAPLUS

CN Morpholine, 4-[2-[4-[2,8-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



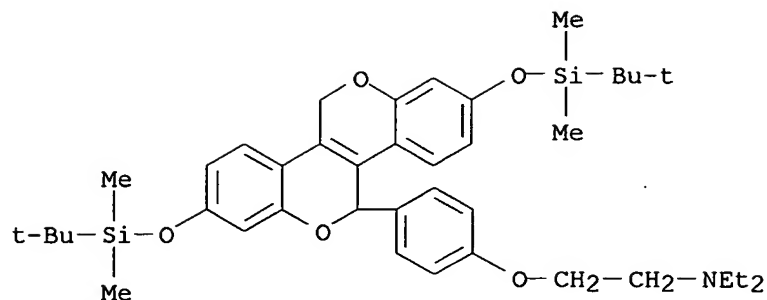
RN 554430-92-1 CAPLUS

CN Pyrrolidine, 1-[2-[4-[2,8-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



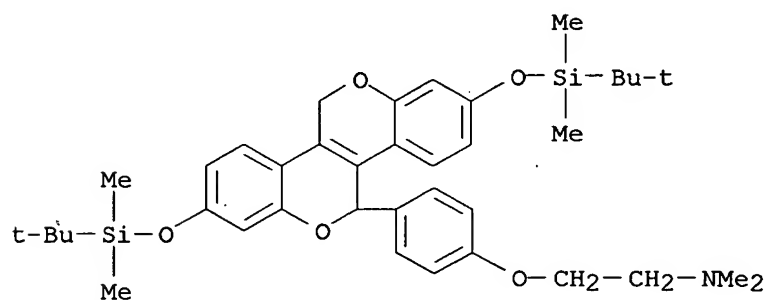
RN 554430-93-2 CAPLUS

CN Ethanamine, 2-[4-[2,8-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]-N,N-diethyl- (9CI) (CA INDEX NAME)



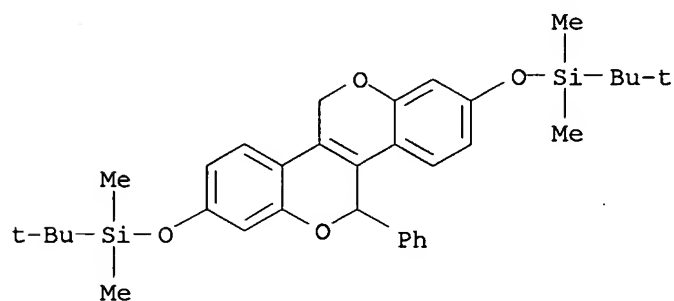
RN 554430-94-3 CAPLUS

CN Ethanamine, 2-[4-[2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]-N,N-dimethyl- (9CI) (CA INDEX NAME)



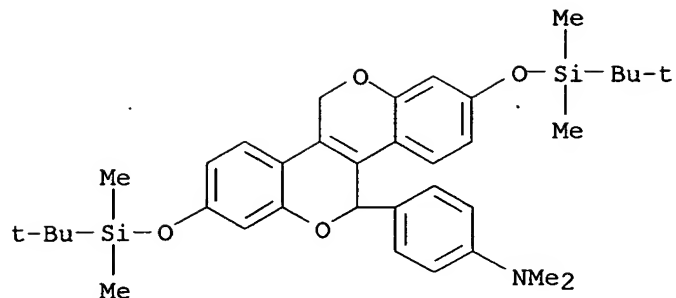
RN 554430-95-4 CAPLUS

CN Silane, [(5,11-dihydro-5-phenyl[1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl)bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



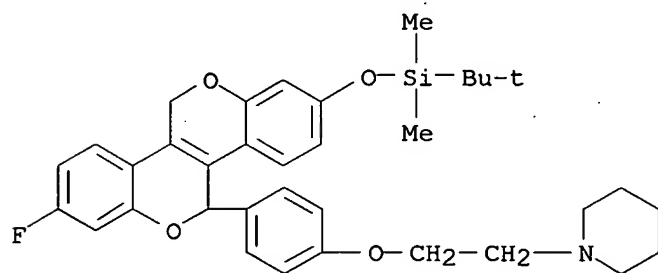
RN 554430-96-5 CAPLUS

CN Benzenamine, 4-[2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



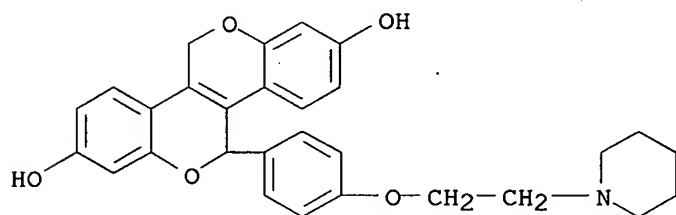
RN 554430-97-6 CAPLUS

CN Piperidine, 1-[2-[4-[2-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-fluoro-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]- (9CI)  
(CA INDEX NAME)



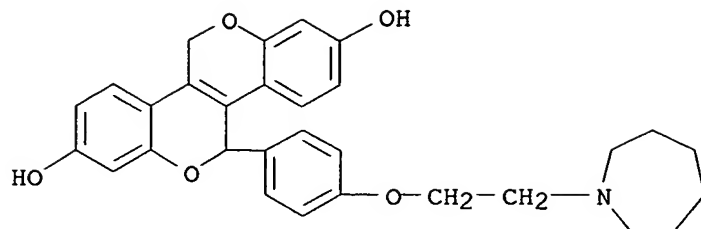
RN 554430-98-7 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



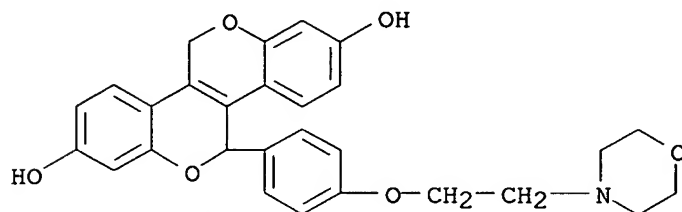
RN 554430-99-8 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-5,11-dihydro- (9CI) (CA INDEX NAME)



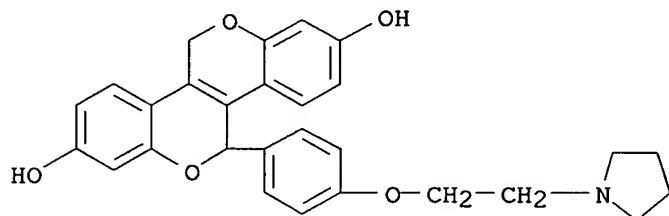
RN 554431-00-4 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-[4-[2-(4-morpholinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



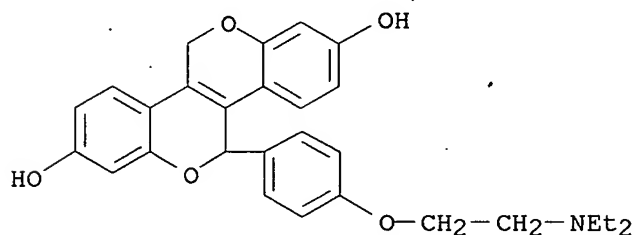
RN 554431-01-5 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-[4-[2-(1-pyrrolidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



RN 554431-02-6 CAPLUS

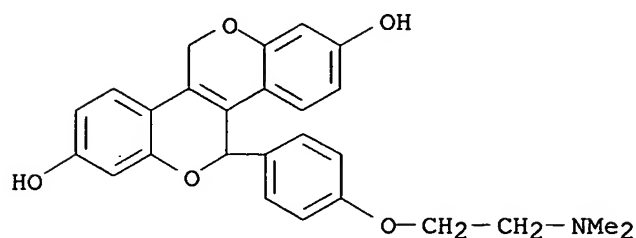
CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5-[4-[2-(diethylamino)ethoxy]phenyl]-5,11-dihydro- (9CI) (CA INDEX NAME)



RN 554431-03-7 CAPLUS

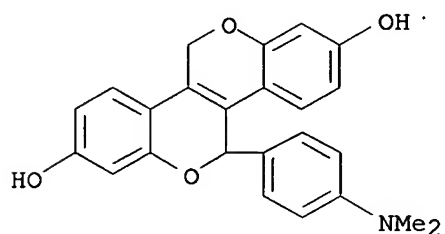
CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5-[4-[2-

(dimethylamino)ethoxy]phenyl]-5,11-dihydro- (9CI) (CA INDEX NAME)



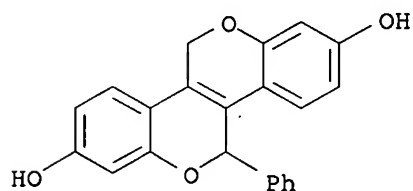
RN 554431-04-8 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5-[4-(dimethylamino)phenyl]-5,11-dihydro- (9CI) (CA INDEX NAME)



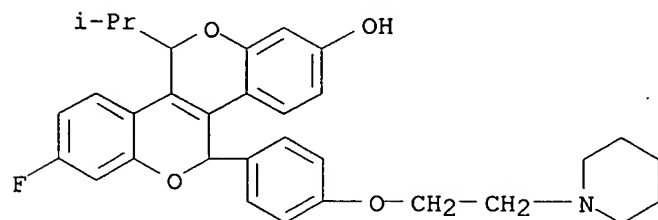
RN 554431-05-9 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5-phenyl- (9CI) (CA INDEX NAME)



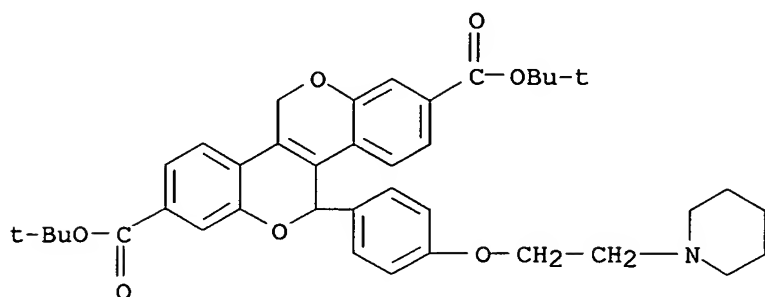
RN 554431-06-0 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2-ol, 8-fluoro-5,11-dihydro-11-(1-methylethyl)-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



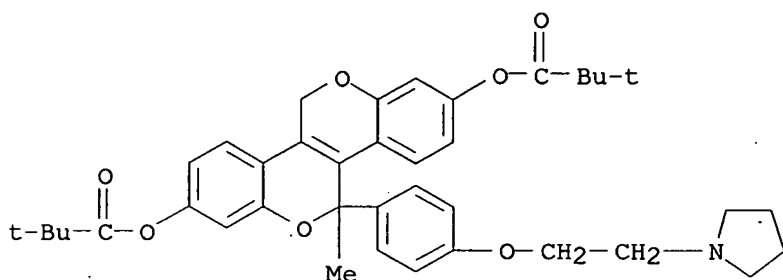
RN 554431-07-1 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-dicarboxylic acid,  
5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, bis(1,1-  
dimethylethyl) ester (9CI) (CA INDEX NAME)



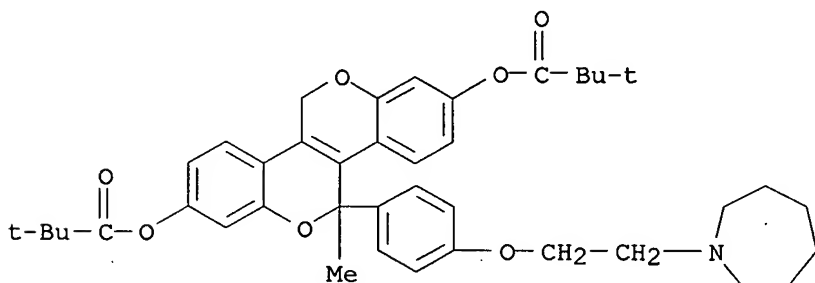
RN 554431-08-2 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 5,11-dihydro-5-methyl-5-[4-[2-(1-pyrrolidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl ester (9CI) (CA INDEX NAME)



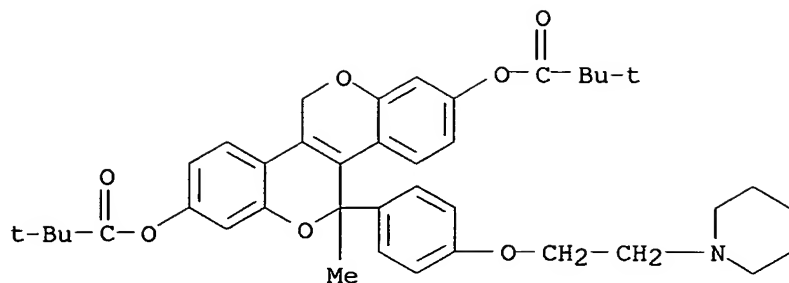
RN 554431-09-3 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-5,11-dihydro-5-methyl[1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl ester (9CI) (CA INDEX NAME)



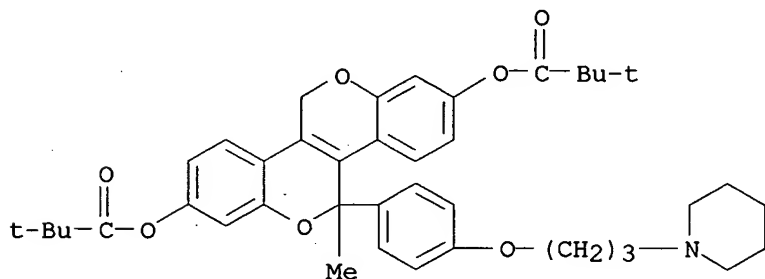
RN 554431-10-6 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 5,11-dihydro-5-methyl-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl ester (9CI) (CA INDEX NAME)



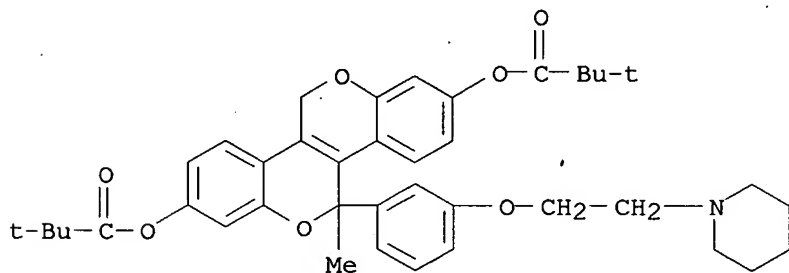
RN 554431-11-7 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 5,11-dihydro-5-methyl-5-[4-[3-(1-piperidinyl)propoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl ester (9CI) (CA INDEX NAME)



RN 554431-12-8 CAPLUS

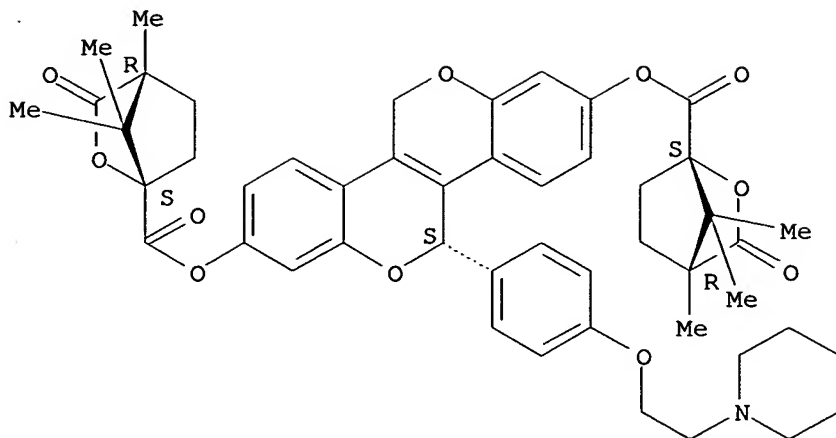
CN Propanoic acid, 2,2-dimethyl-, 5,11-dihydro-5-methyl-5-[3-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl ester (9CI) (CA INDEX NAME)



RN 554431-13-9 CAPLUS

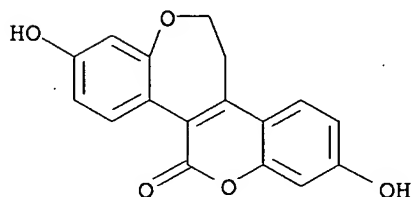
CN 2-Oxabicyclo[2.2.1]heptane-1-carboxylic acid, 4,7,7-trimethyl-3-oxo-, (5S)-5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl ester, (1S,1'S,4R,4'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



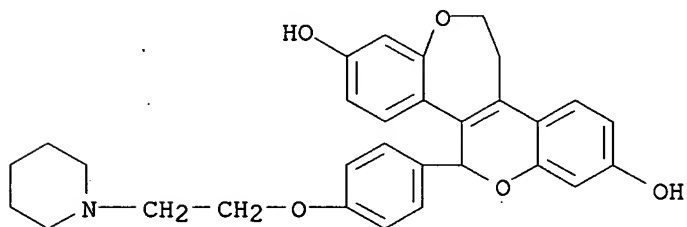
RN 554431-14-0 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 11,12-dihydro-2,8-dihydroxy-  
(9CI) (CA INDEX NAME)



RN 554431-15-1 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 11,12-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)

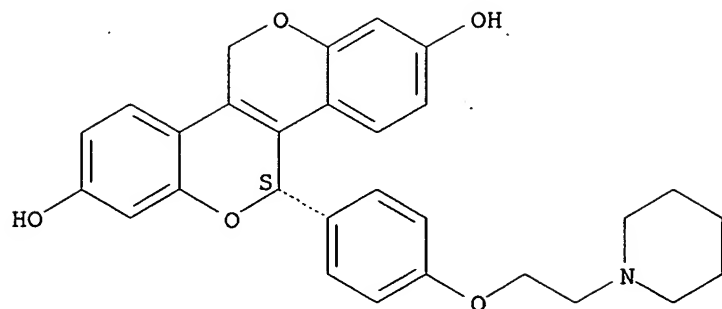


RN 554431-16-2 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

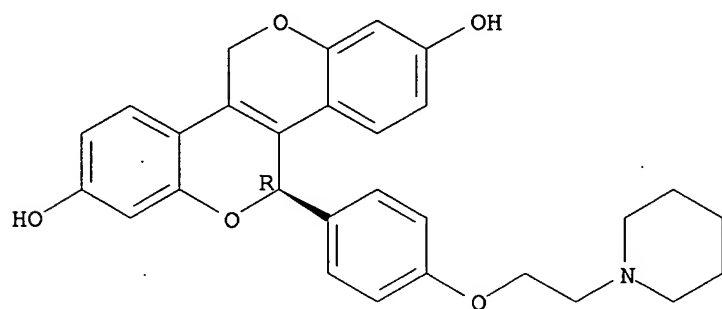




RN 554431-17-3 CAPLUS

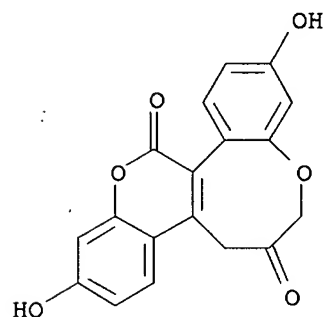
CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



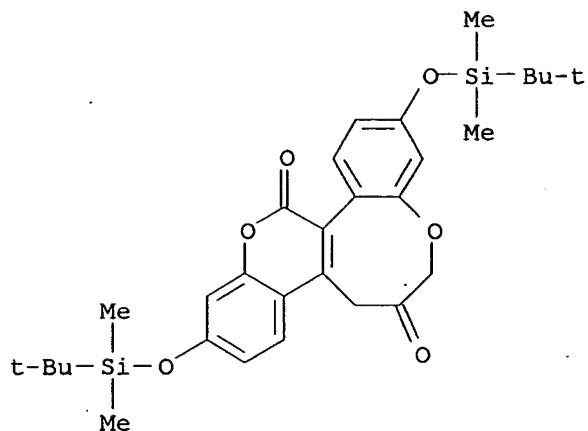
RN 554431-18-4 CAPLUS

CN [1]Benzopyrano[4,3-e][1]benzoxocin-6,13(5H,7H)-dione, 2,10-dihydroxy- (9CI) (CA INDEX NAME)



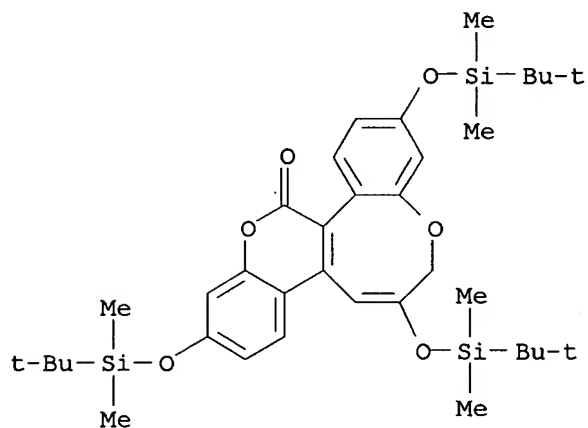
RN 554431-19-5 CAPLUS

CN [1]Benzopyrano[4,3-e][1]benzoxocin-6,13(5H,7H)-dione, 2,10-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]- (9CI) (CA INDEX NAME)



RN 554431-20-8 CAPLUS

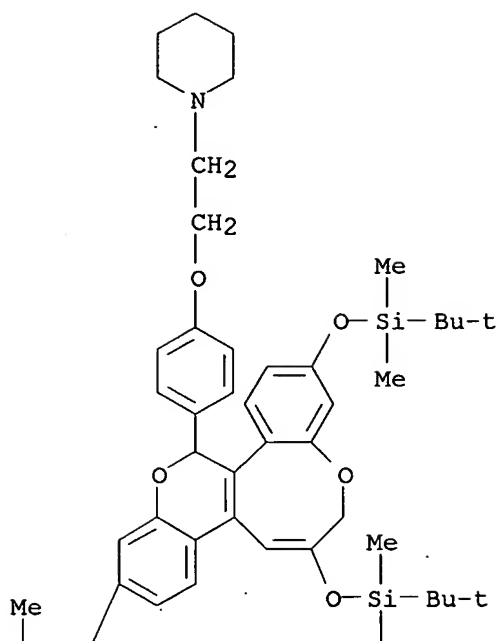
CN [1]Benzopyrano[4,3-e][1]benzoxocin-13(7H)-one, 2,6,10-tris[[(1,1-dimethylethyl)dimethylsilyl]oxy]- (9CI) (CA INDEX NAME)



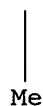
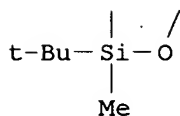
RN 554431-21-9 CAPLUS

CN Piperidine, 1-[2-[4-[2,6,10-tris[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7,13-dihydro[1]benzopyrano[4,3-e][1]benzoxocin-13-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

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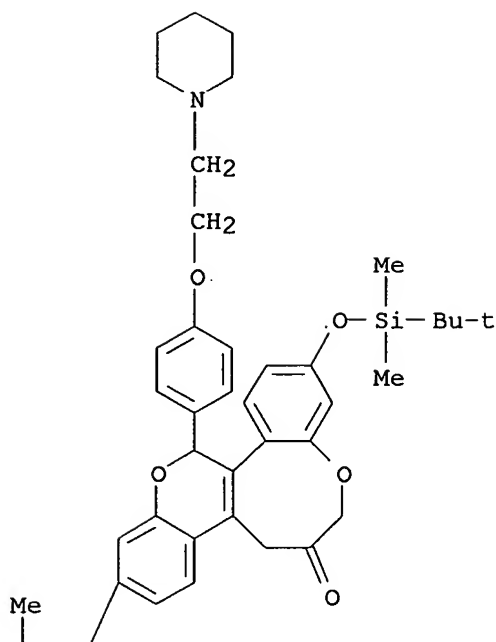


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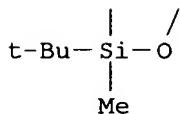


RN 554431-22-0 CAPLUS  
 CN [1]Benzopyrano[4,3-e][1]benzoxocin-6(7H)-one, 2,10-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,13-dihydro-13-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)

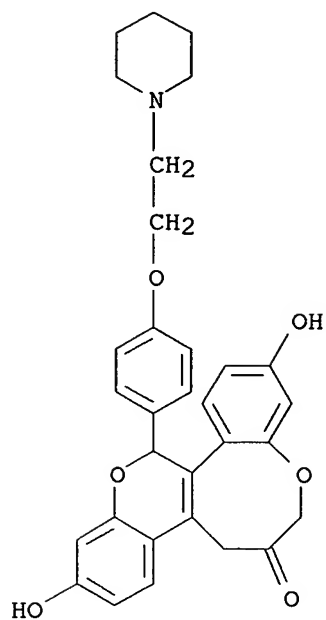
PAGE 1-A



PAGE 2-A

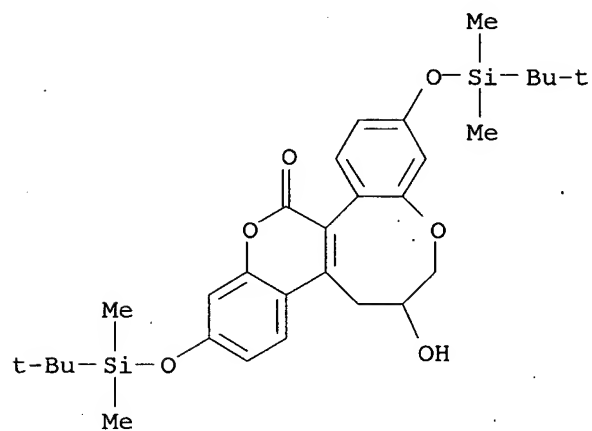


RN 554431-23-1 CAPLUS  
 CN [1]Benzopyrano[4,3-e][1]benzoxocin-6(7H)-one, 5,13-dihydro-2,10-dihydroxy-  
 13-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



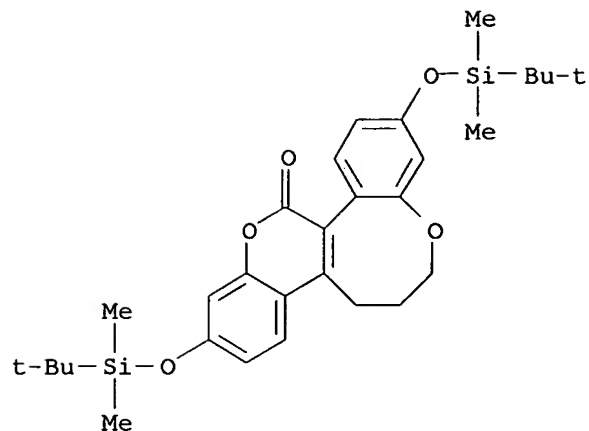
RN 554431-24-2 CAPLUS

CN [1]Benzopyrano[4,3-e][1]benzoxocin-13(5H)-one, 2,10-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6,7-dihydro-6-hydroxy- (9CI) (CA INDEX NAME)



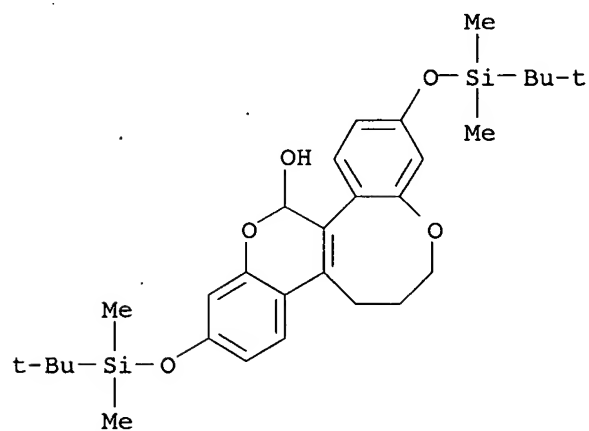
RN 554431-25-3 CAPLUS

CN [1]Benzopyrano[4,3-e][1]benzoxocin-13(5H)-one, 2,10-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6,7-dihydro- (9CI) (CA INDEX NAME)



RN 554431-26-4 CAPLUS

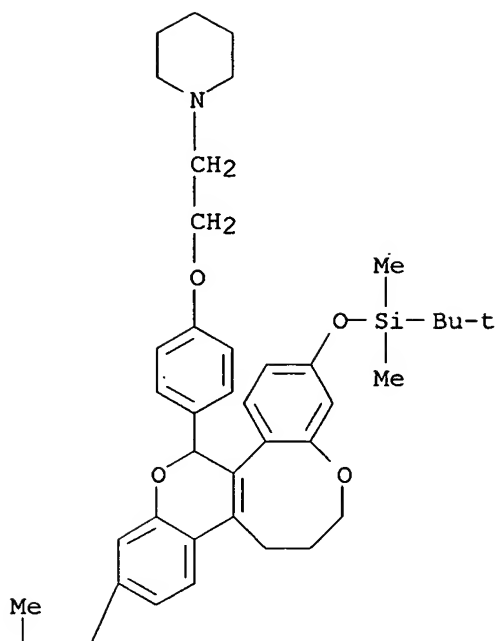
CN [1]Benzopyrano[4,3-e][1]benzoxocin-13-ol, 2,10-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,6,7,13-tetrahydro- (9CI) (CA INDEX NAME)



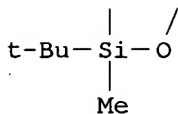
RN 554431-27-5 CAPLUS

CN Piperidine, 1-[2-[4-[2,10-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,6,7,13-tetrahydro[1]benzopyrano[4,3-e][1]benzoxocin-13-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

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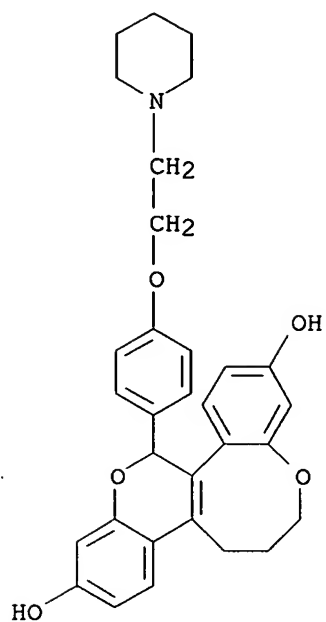


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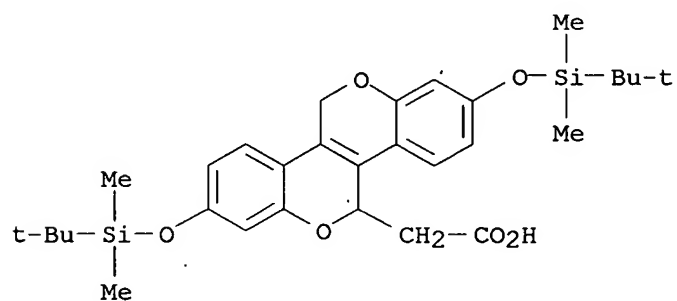
RN 554431-28-6 CAPLUS

CN [1]Benzopyrano[4,3-e][1]benzoxocin-2,10-diol, 5,6,7,13-tetrahydro-13-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



RN 554431-29-7 CAPLUS

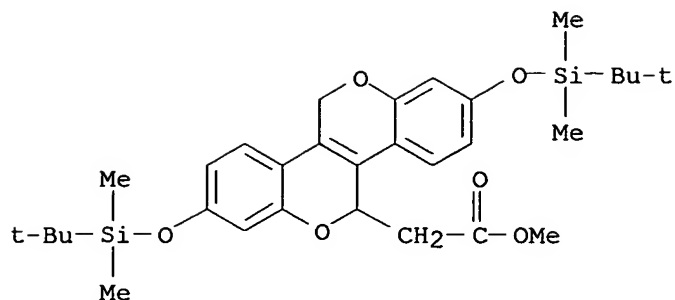
CN [1]Benzopyrano[4,3-c][1]benzopyran-5-acetic acid, 2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro- (9CI) (CA INDEX NAME)



RN 554431-30-0 CAPLUS

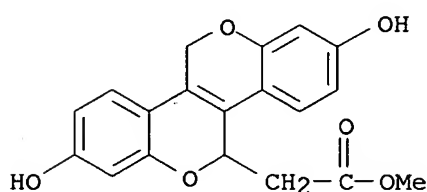
CN [1]Benzopyrano[4,3-c][1]benzopyran-5-acetic acid, 2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro-, methyl ester (9CI) (CA INDEX NAME)





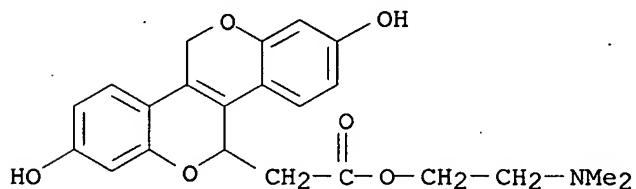
RN 554431-31-1 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5-acetic acid, 5,11-dihydro-2,8-dihydroxy-, methyl ester (9CI) (CA INDEX NAME)



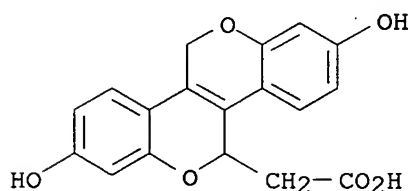
RN 554431-32-2 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5-acetic acid, 5,11-dihydro-2,8-dihydroxy-, 2-(dimethylamino)ethyl ester (9CI) (CA INDEX NAME)



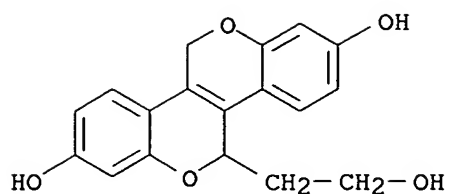
RN 554431-33-3 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5-acetic acid, 5,11-dihydro-2,8-dihydroxy- (9CI) (CA INDEX NAME)



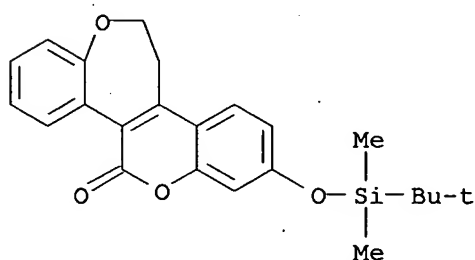
RN 554431-34-4 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)



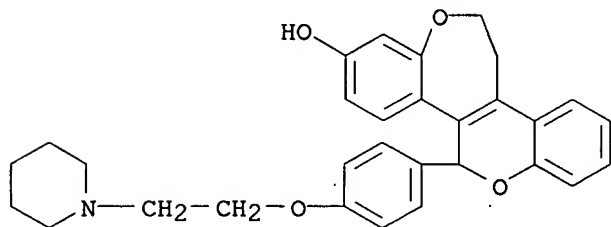
RN 554431-35-5 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 8-[[1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro- (9CI) (CA INDEX NAME)



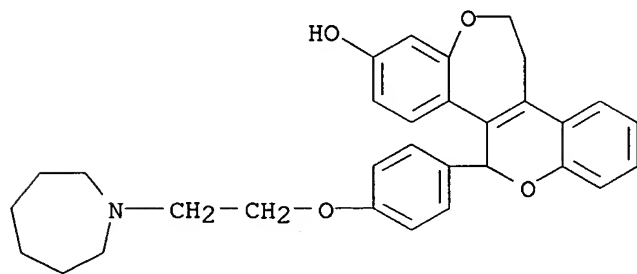
RN 554431-36-6 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 11,12-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)

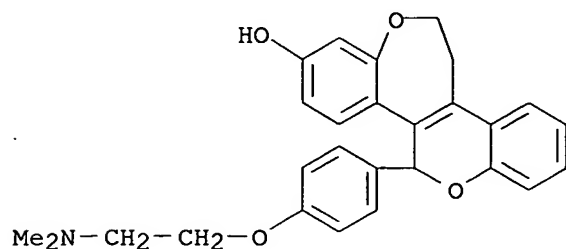


RN 554431-37-7 CAPLUS

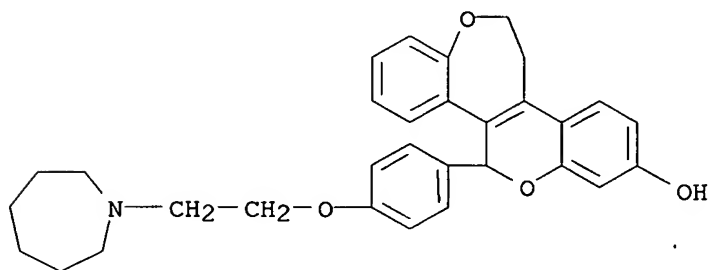
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro- (9CI) (CA INDEX NAME)



RN 554431-38-8 CAPLUS  
 CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 5-[4-[2-(dimethylamino)ethoxy]phenyl]-11,12-dihydro- (9CI) (CA INDEX NAME)

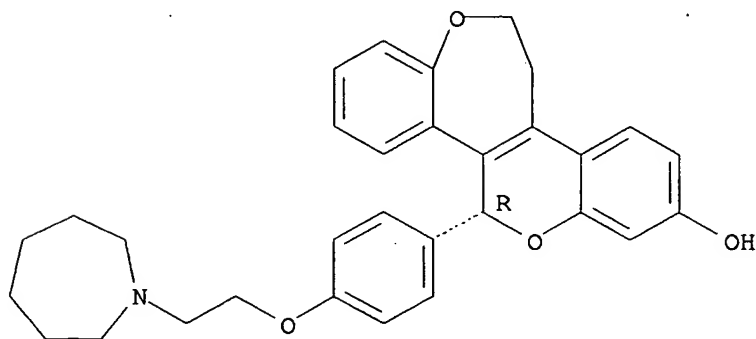


RN 554431-39-9 CAPLUS  
 CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-8-ol, 5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro- (9CI) (CA INDEX NAME)



RN 554431-40-2 CAPLUS  
 CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-8-ol, 5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro-, (5R)- (9CI) (CA INDEX NAME)

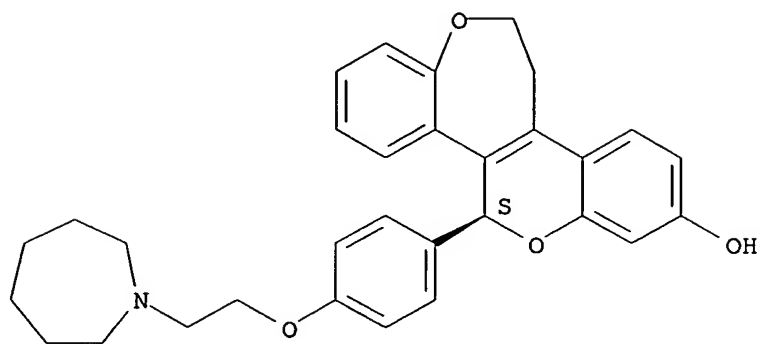
Absolute stereochemistry. Rotation (+).



RN 554431-41-3 CAPLUS  
 CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-8-ol, 5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro-, (5S)- (9CI) (CA INDEX NAME)

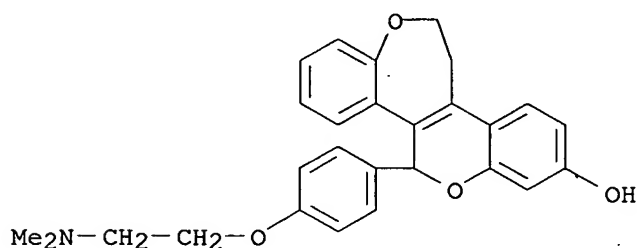
10/307,735

Absolute stereochemistry. Rotation (-).



RN 554431-42-4 CAPLUS

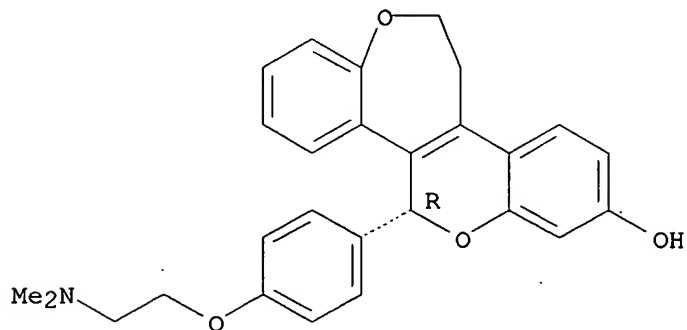
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-8-ol, 5-[4-[2-(dimethylamino)ethoxy]phenyl]-11,12-dihydro- (9CI) (CA INDEX NAME)



RN 554431-43-5 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-8-ol, 5-[4-[2-(dimethylamino)ethoxy]phenyl]-11,12-dihydro-, (5R)- (9CI) (CA INDEX NAME)

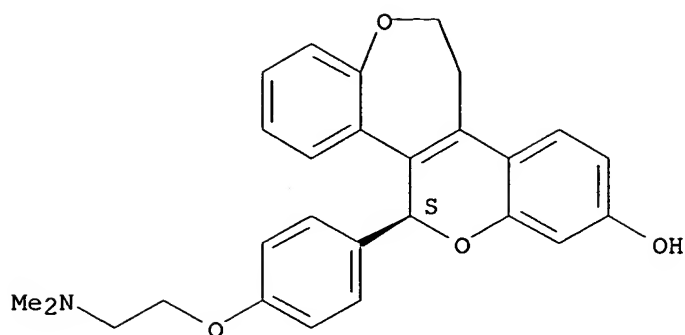
Absolute stereochemistry. Rotation (+).



RN 554431-44-6 CAPLUS

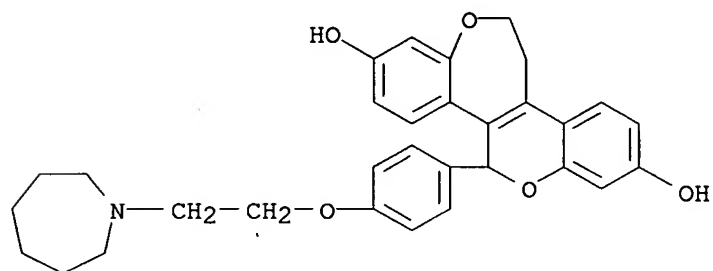
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-8-ol, 5-[4-[2-(dimethylamino)ethoxy]phenyl]-11,12-dihydro-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 554431-45-7 CAPLUS

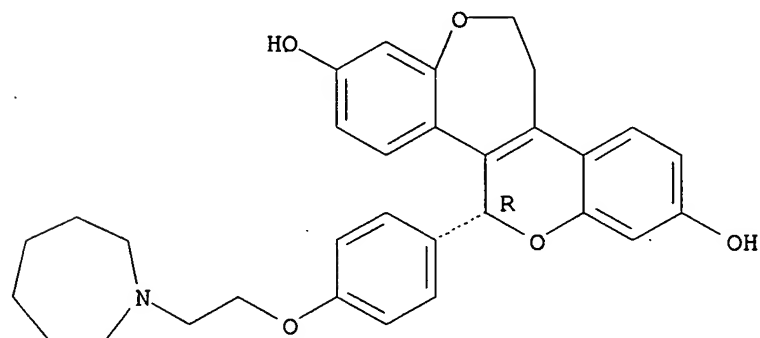
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro- (9CI) (CA INDEX NAME)



RN 554431-46-8 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 5-[4-[2-(octahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro-, (5R)- (9CI) (CA INDEX NAME)

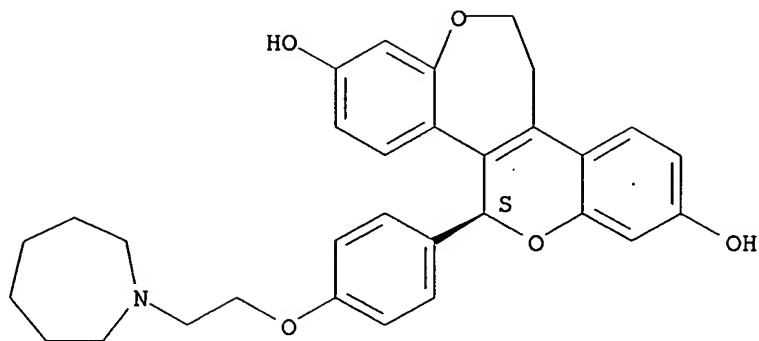
Absolute stereochemistry. Rotation (+).



RN 554431-47-9 CAPLUS

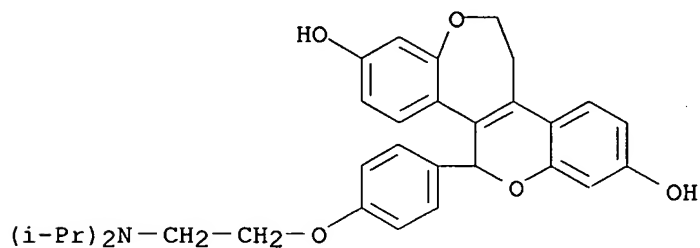
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 5-[4-[2-(octahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 554431-48-0 CAPLUS

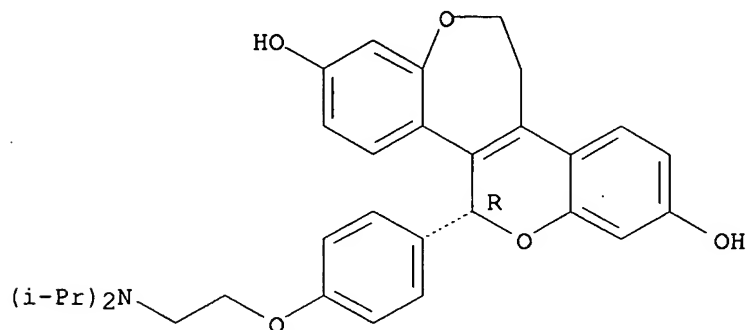
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 5-[4-[2-[bis(1-methylethyl)amino]ethoxy]phenyl]-11,12-dihydro- (9CI) (CA INDEX NAME)



RN 554431-49-1 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 5-[4-[2-[bis(1-methylethyl)amino]ethoxy]phenyl]-11,12-dihydro-; (5R)- (9CI) (CA INDEX NAME)

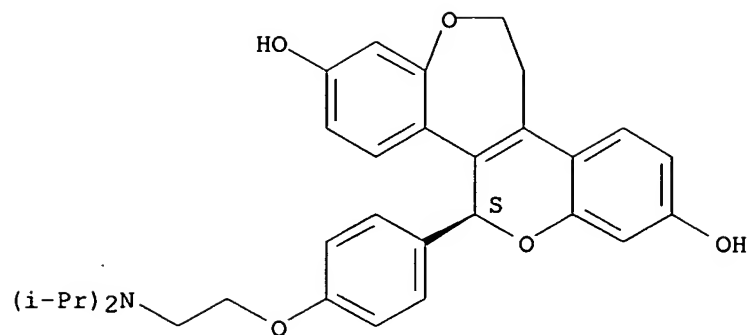
Absolute stereochemistry. Rotation (+).



RN 554431-50-4 CAPLUS

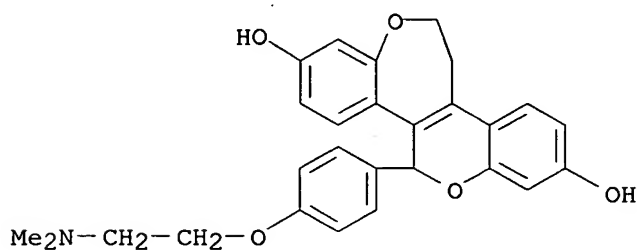
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 5-[4-[2-[bis(1-methylethyl)amino]ethoxy]phenyl]-11,12-dihydro-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 554431-51-5 CAPLUS

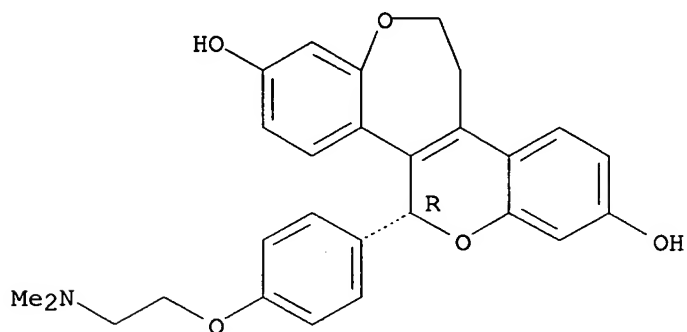
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 5-[4-[2-(dimethylamino)ethoxy]phenyl]-11,12-dihydro- (9CI) (CA INDEX NAME)



RN 554431-52-6 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 5-[4-[2-(dimethylamino)ethoxy]phenyl]-11,12-dihydro-, (5R)- (9CI) (CA INDEX NAME)

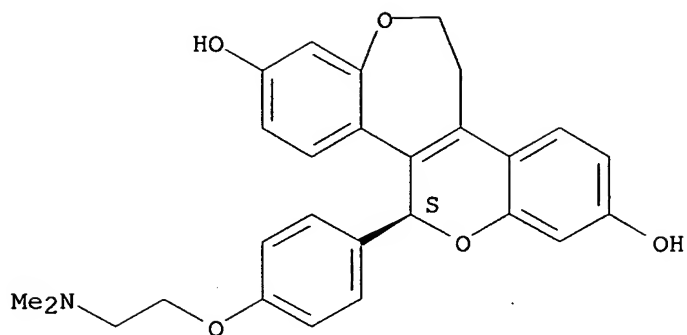
Absolute stereochemistry. Rotation (+).



RN 554431-53-7 CAPLUS

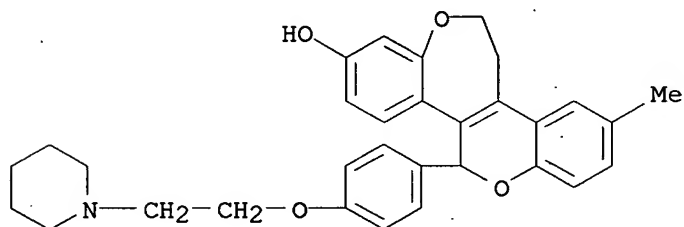
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 5-[4-[2-(dimethylamino)ethoxy]phenyl]-11,12-dihydro-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



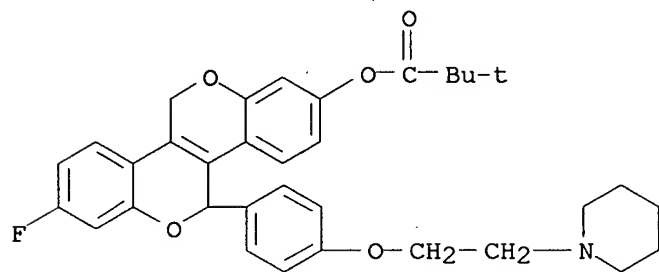
RN 554431-54-8 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 11,12-dihydro-9-methyl-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



RN 554431-55-9. CAPLUS

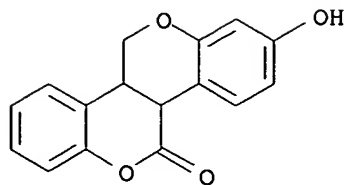
CN Propanoic acid, 2,2-dimethyl-, 8-fluoro-5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2-yl ester (9CI) (CA INDEX NAME)



RN 554431-56-0 CAPLUS

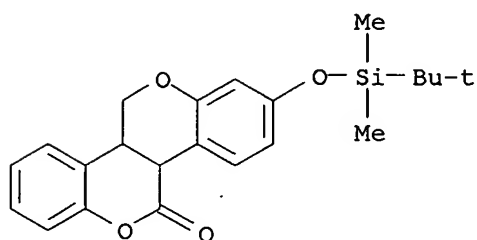
CN [1]Benzopyrano[4,3-c][1]benzopyran-5(4bH)-one, 10b,11-dihydro-2-hydroxy- (9CI) (CA INDEX NAME)





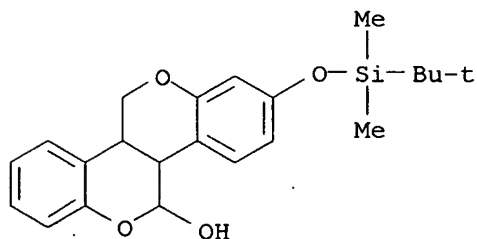
RN 554431-57-1 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5(4bH)-one, 2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-10b,11-dihydro- (9CI) (CA INDEX NAME)



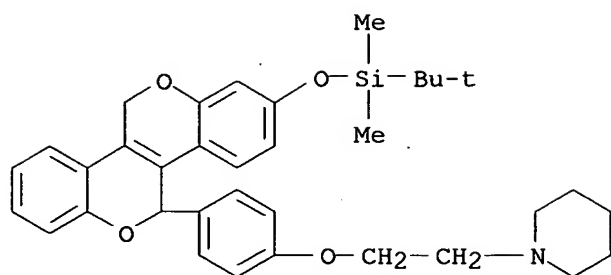
RN 554431-58-2 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5-ol, 2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4b,5,10b,11-tetrahydro- (9CI) (CA INDEX NAME)



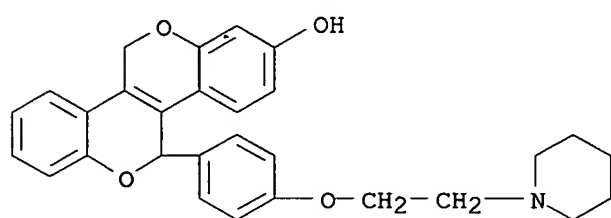
RN 554431-59-3 CAPLUS

CN Piperidine, 1-[2-[4-[2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



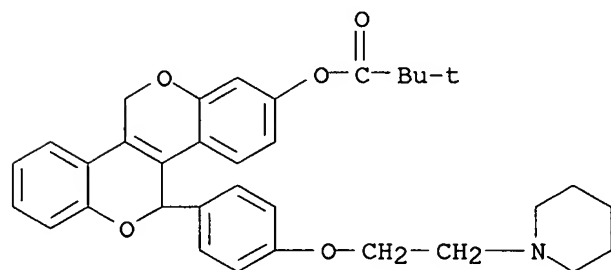
RN 554431-60-6 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2-ol, 5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



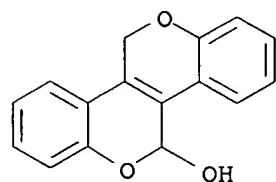
RN 554431-61-7 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2-yl ester (9CI) (CA INDEX NAME)



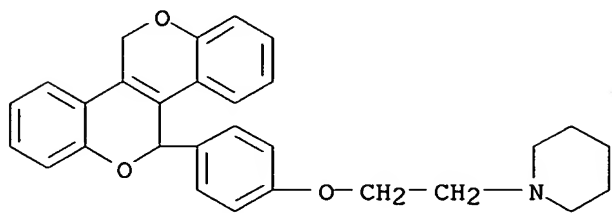
RN 554431-62-8 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5-ol, 5,11-dihydro- (9CI) (CA INDEX NAME)



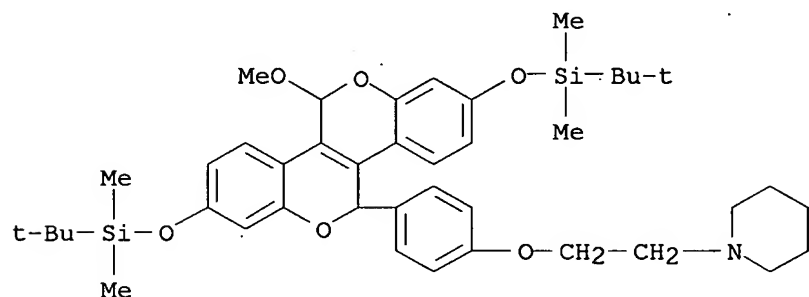
RN 554431-63-9 CAPLUS

CN Piperidine, 1-[2-[4-(5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl)phenoxy]ethyl]- (9CI) (CA INDEX NAME)



RN 554431-64-0 CAPLUS

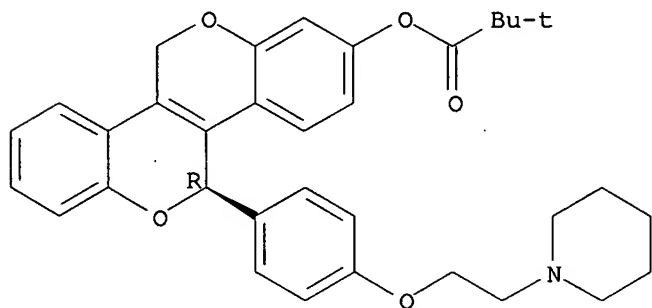
CN Piperidine, 1-[2-[4-[2,8-bis[[ (1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro-11-methoxy[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



RN 554431-65-1 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, (5R)-5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

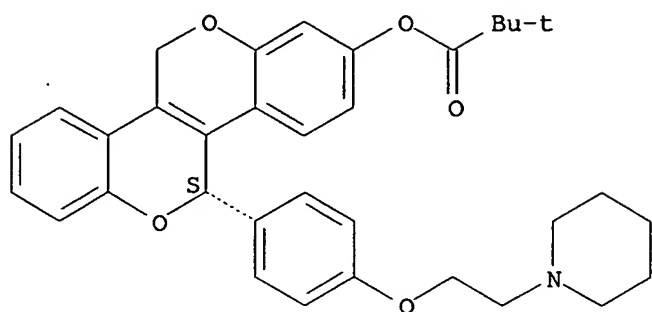


RN 554431-66-2 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, (5S)-5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2-yl ester (9CI) (CA INDEX NAME)

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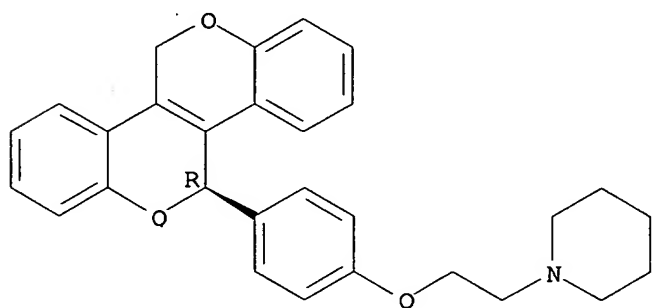
Absolute stereochemistry. Rotation (+).



RN 554431-67-3 CAPLUS

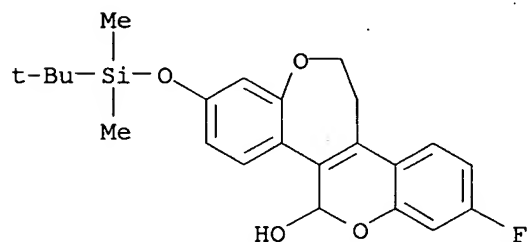
CN Piperidine, 1-[2-[4-[(5R)-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 554431-68-4 CAPLUS

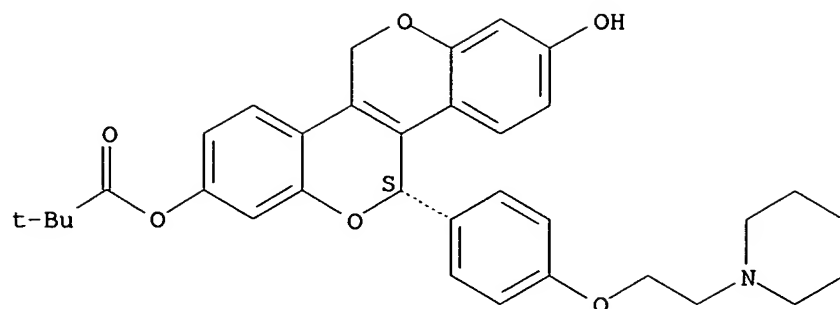
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-ol, 2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-fluoro-11,12-dihydro- (9CI) (CA INDEX NAME)



RN 554431-69-5 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, (11S)-5,11-dihydro-8-hydroxy-11-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2-yl ester (9CI) (CA INDEX NAME)

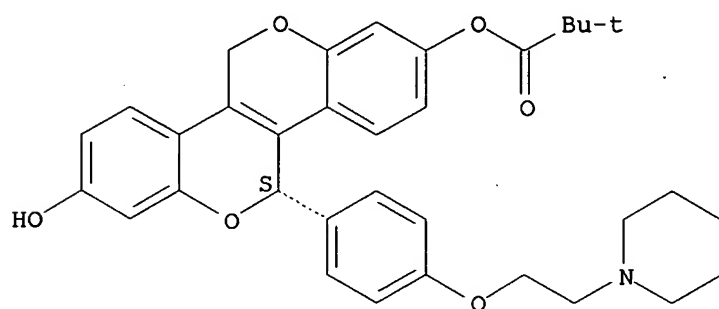
Absolute stereochemistry. Rotation (+).



RN 554431-70-8 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, (5S)-5,11-dihydro-8-hydroxy-5-[4-[3-(1-piperidinyl)propoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2-yl ester (9CI) (CA INDEX NAME)

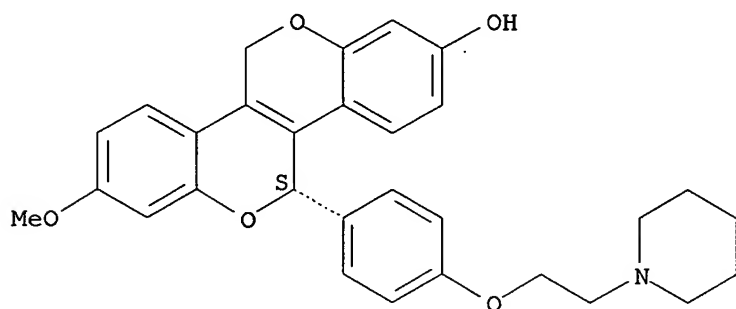
Absolute stereochemistry. Rotation (+).



RN 554431-71-9 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2-ol, 5,11-dihydro-8-methoxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (5S)- (9CI) (CA INDEX NAME)

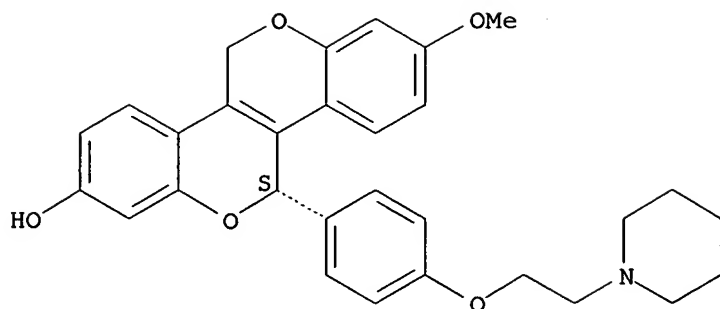
Absolute stereochemistry.



RN 554431-72-0 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2-ol, 5,11-dihydro-8-methoxy-11-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (11S)- (9CI) (CA INDEX NAME)

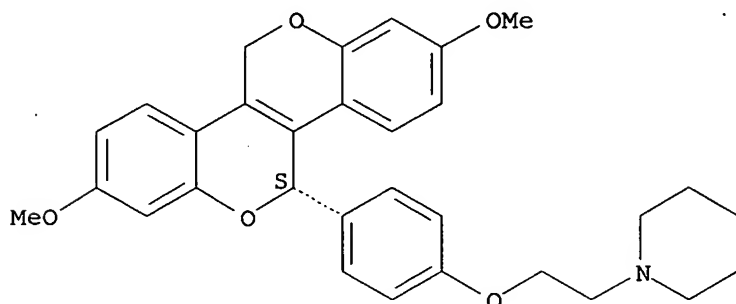
Absolute stereochemistry. Rotation (-).



RN 554431-73-1 CAPLUS

CN Piperidine, 1-[2-[4-[(5S)-5,11-dihydro-2,8-dimethoxy[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

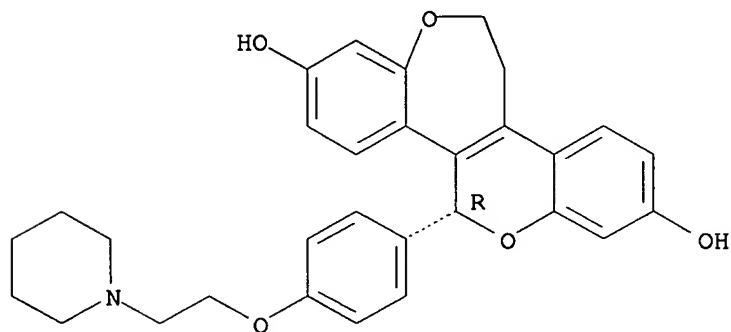
Absolute stereochemistry. Rotation (+).



RN 554431-74-2 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 11,12-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (5R)- (9CI) (CA INDEX NAME)

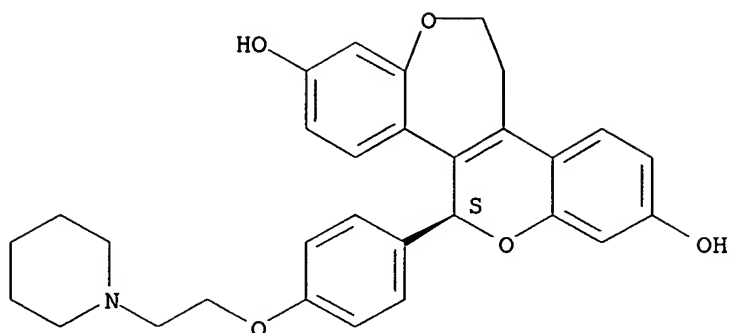
Absolute stereochemistry. Rotation (+).



RN 554431-75-3 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 11,12-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (5S)- (9CI) (CA INDEX NAME)

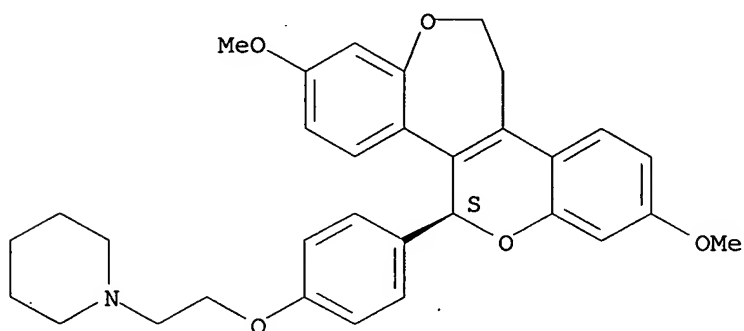
Absolute stereochemistry. Rotation (-).



RN 554431-76-4 CAPLUS

CN Piperidine, 1-[2-[4-[(5S)-11,12-dihydro-2,8-dimethoxy-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

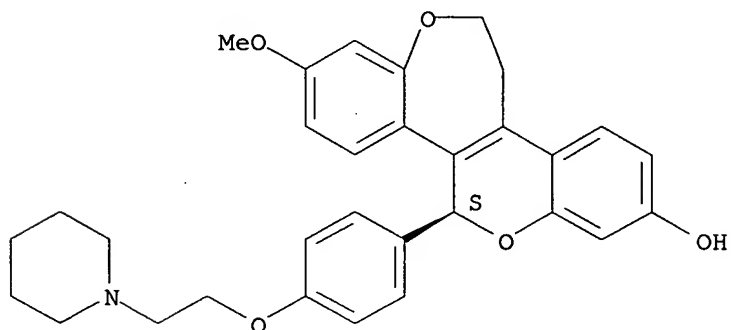
Absolute stereochemistry. Rotation (-).



RN 554431-77-5 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-8-ol, 11,12-dihydro-2-methoxy-5-[4-(2-(1-piperidinyl)ethoxy)phenyl]-, (5S)- (9CI) (CA INDEX NAME)

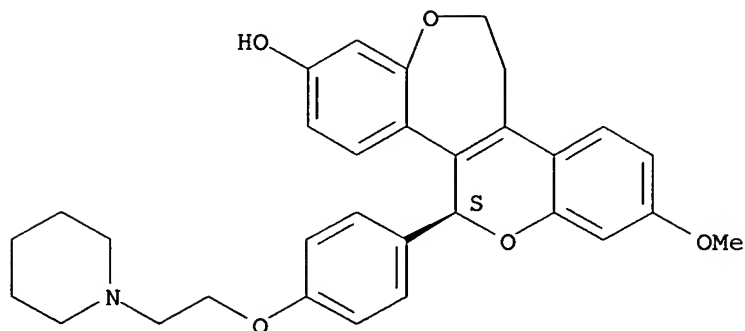
Absolute stereochemistry. Rotation (-).



RN 554431-78-6 CAPLUS

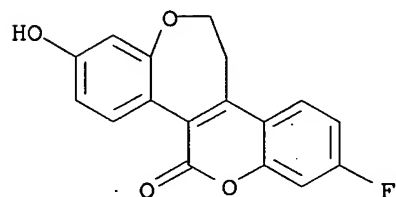
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 11,12-dihydro-8-methoxy-5-[4-(2-(1-piperidinyl)ethoxy)phenyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



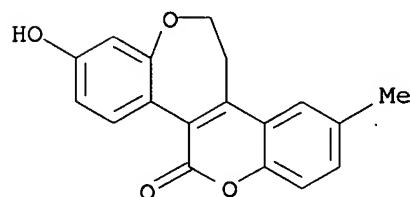
RN 554431-79-7 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 8-fluoro-11,12-dihydro-2-hydroxy- (9CI) (CA INDEX NAME)



RN 554431-80-0 CAPLUS

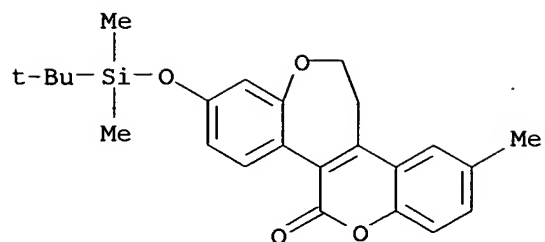
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 11,12-dihydro-2-hydroxy-9-methyl- (9CI) (CA INDEX NAME)



RN 554431-81-1 CAPLUS

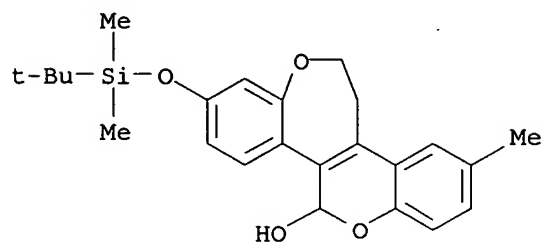
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro-9-methyl- (9CI) (CA INDEX NAME)





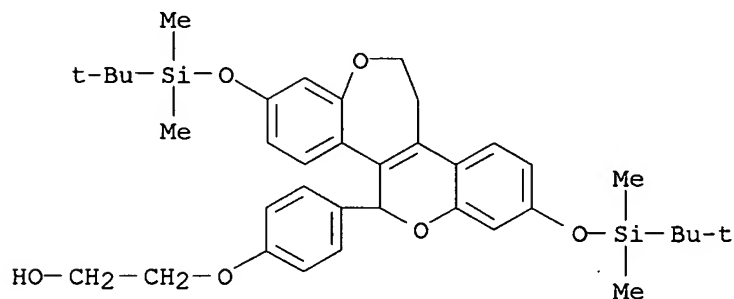
RN 554431-82-2 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-ol, 2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro-9-methyl- (9CI) (CA INDEX NAME)



RN 554431-83-3 CAPLUS

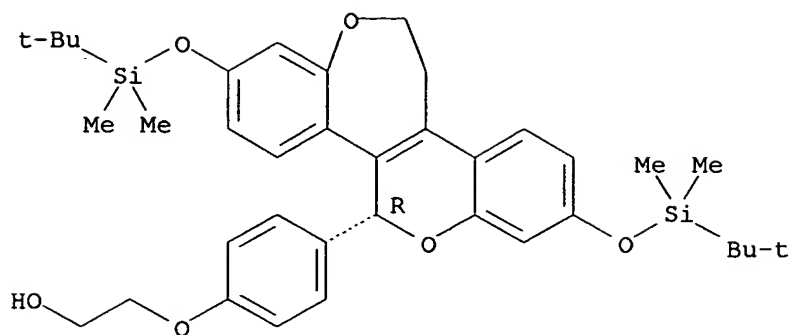
CN Ethanol, 2-[4-[2,8-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]- (9CI) (CA INDEX NAME)



RN 554431-84-4 CAPLUS

CN Ethanol, 2-[4-[(5R)-2,8-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]- (9CI) (CA INDEX NAME)

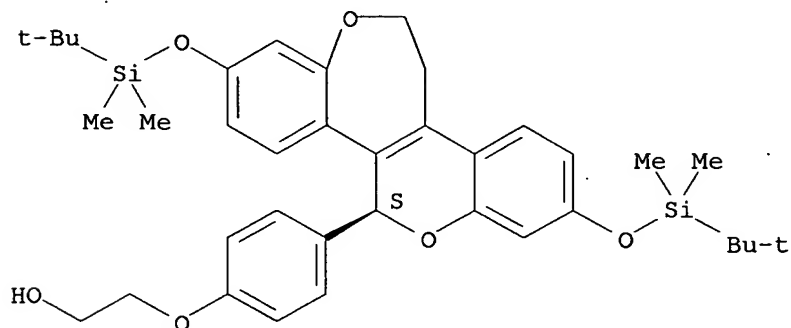
Absolute stereochemistry. Rotation (+).



RN 554431-85-5 CAPLUS

CN Ethanol, 2-[4-[(5S)-2,8-bis[[ (1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]- (9CI) (CA INDEX NAME)

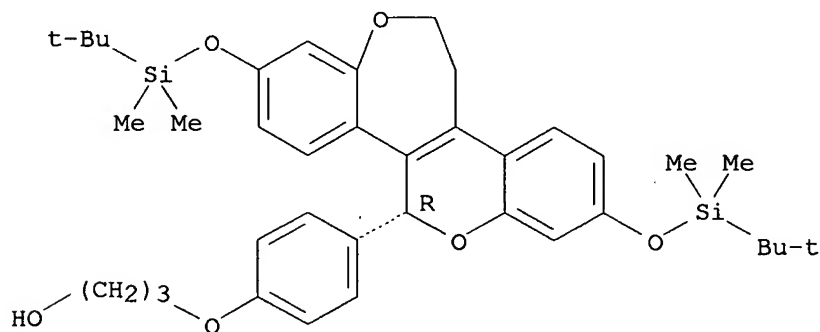
Absolute stereochemistry. Rotation (-).



RN 554431-86-6 CAPLUS

CN 1-Propanol, 3-[4-[(5R)-2,8-bis[[ (1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

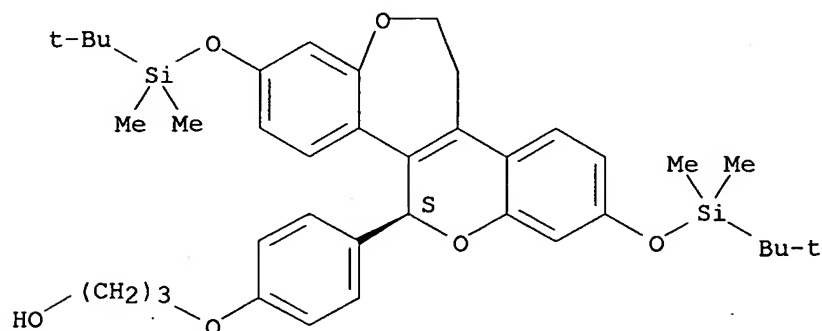


RN 554431-87-7 CAPLUS

10/307,735

CN 1-Propanol, 3-[4-[(5S)-2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]- (9CI)  
(CA INDEX NAME)

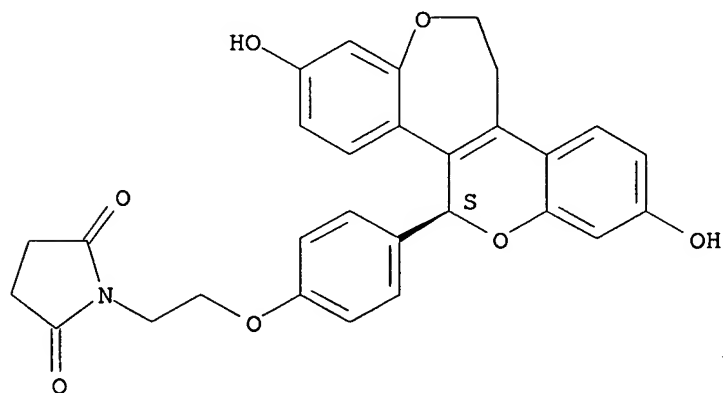
Absolute stereochemistry. Rotation (-).



RN 554431-88-8 CAPLUS

CN 2,5-Pyrrolidinedione, 1-[2-[4-[(5S)-11,12-dihydro-2,8-dihydroxy-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

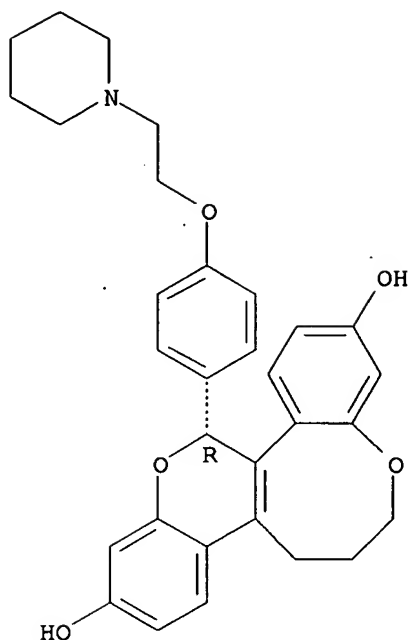
Absolute stereochemistry. Rotation (+).



RN 554431-92-4 CAPLUS

CN [1]Benzopyrano[4,3-e][1]benzoxocin-2,10-diol, 5,6,7,13-tetrahydro-13-[4-[2-(1-piperidinyl)ethoxy]phenyl]-; (13R)- (9CI) (CA INDEX NAME)

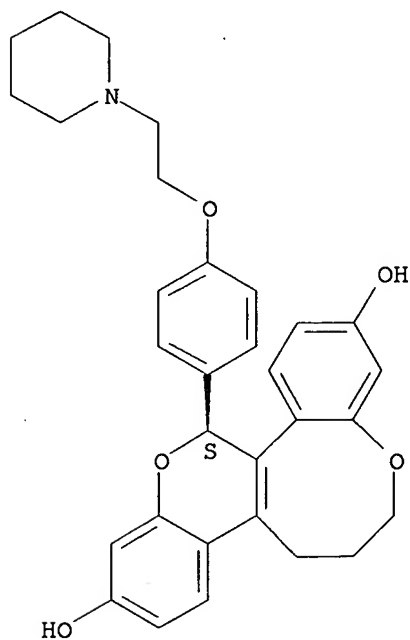
Absolute stereochemistry. Rotation (-).



RN 554431-93-5 CAPLUS

CN [1]Benzopyrano[4,3-e][1]benzoxocin-2,10-diol, 5,6,7,13-tetrahydro-13-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (13S)- (9CI) (CA INDEX NAME)

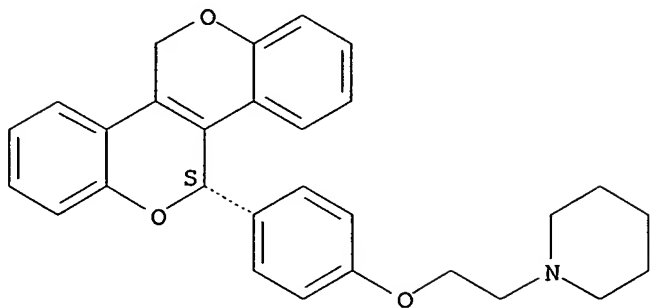
Absolute stereochemistry. Rotation (+).



RN 554433-05-5 CAPLUS

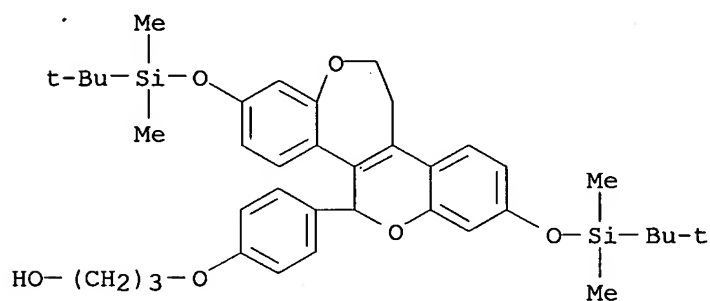
CN Piperidine, 1-[2-[4-[(5S)-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 554433-06-6 CAPLUS

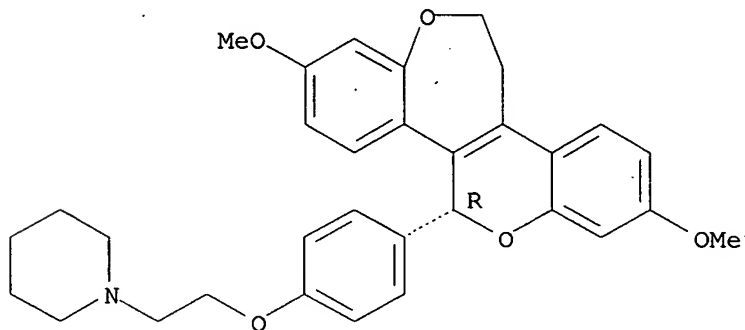
CN 1-Propanol, 3-[4-[2,8-bis[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]- (9CI) (CA INDEX NAME)



RN 810668-60-1 CAPLUS

CN Piperidine, 1-[2-[4-[(12R)-5,12-dihydro-2,9-dimethoxy-6H-[1]benzopyrano[4,3-d][1]benzoxepin-12-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

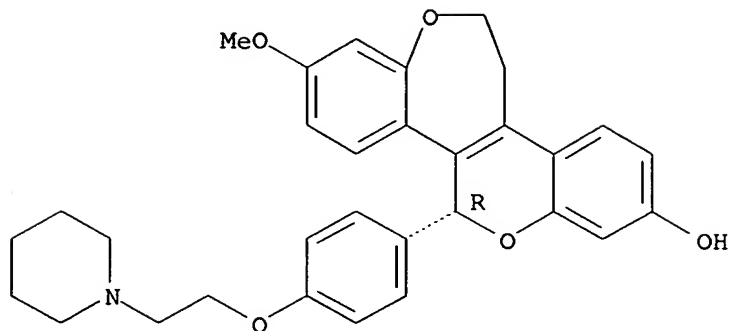
Absolute stereochemistry. Rotation (+).



RN 810668-61-2 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-8-ol, 11,12-dihydro-2-methoxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (5R)- (9CI) (CA INDEX NAME)

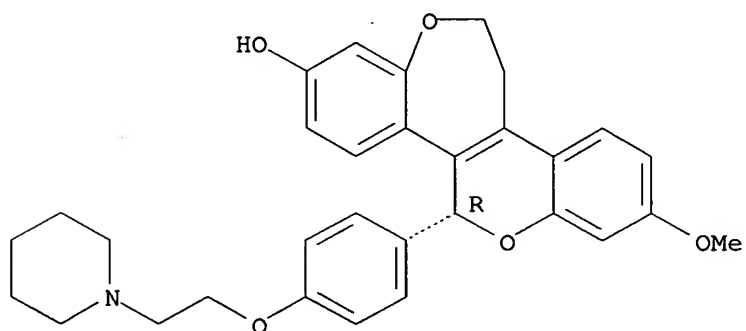
Absolute stereochemistry. Rotation (+).



RN 810668-62-3 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 11,12-dihydro-8-methoxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (5R)- (9CI) (CA INDEX NAME)

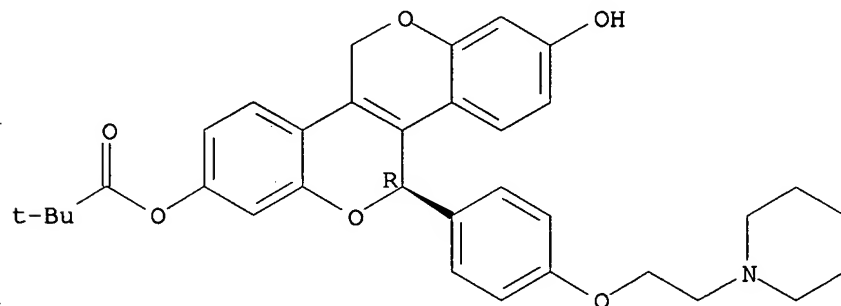
Absolute stereochemistry. Rotation (+).



RN 810668-63-4 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, (11R)-5,11-dihydro-8-hydroxy-11-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2-yl ester (9CI) (CA INDEX NAME)

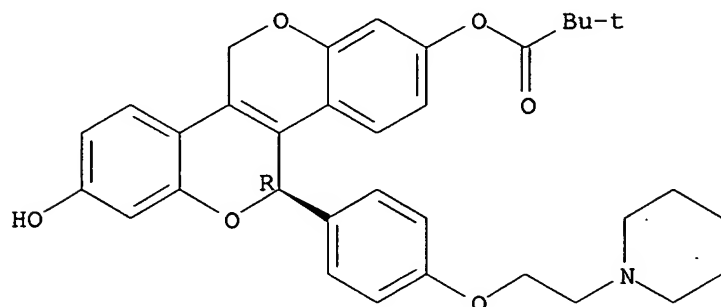
Absolute stereochemistry. Rotation (-).



RN 810668-64-5 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, (5R)-5,11-dihydro-8-hydroxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



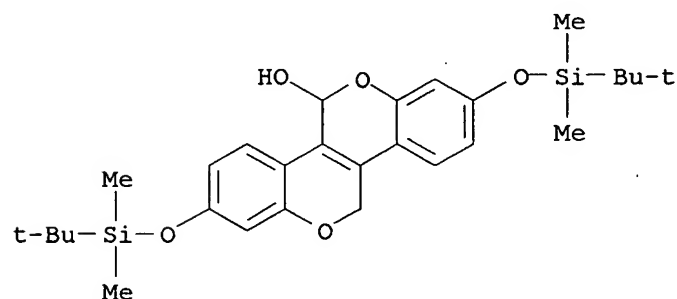
IT 553681-47-3 554430-69-2 554430-70-5  
554430-71-6 554430-72-7 554430-73-8  
554430-74-9 554430-75-0 554430-77-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of tetracyclic heterocycles as selective estrogen receptor modulators (SERMs))

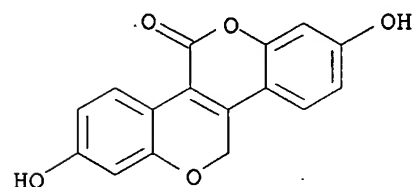
RN 553681-47-3 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5-ol, 2,8-bis[[1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro- (9CI) (CA INDEX NAME)



RN 554430-69-2 CAPLUS

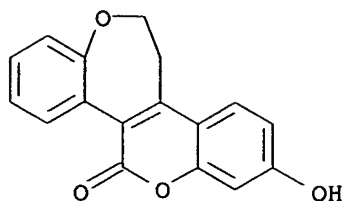
CN [1]Benzopyrano[4,3-c][1]benzopyran-5(11H)-one, 2,8-dihydroxy- (9CI) (CA INDEX NAME)



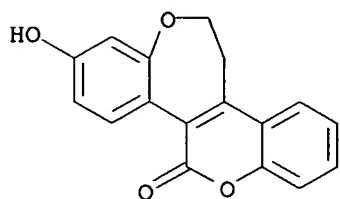
RN 554430-70-5 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 11,12-dihydro-8-hydroxy-

(9CI) (CA INDEX NAME)

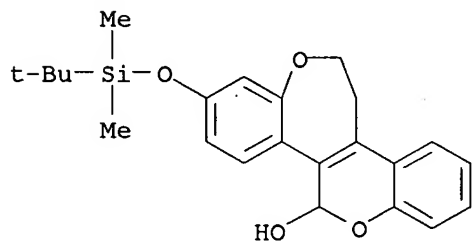


RN 554430-71-6 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 11,12-dihydro-2-hydroxy-  
(9CI) (CA INDEX NAME)

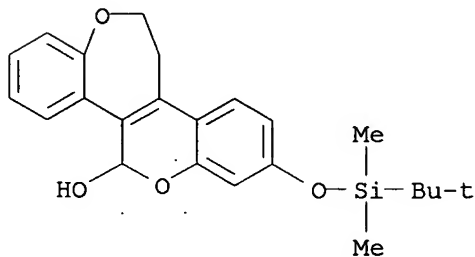
RN 554430-72-7 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-ol, 2-[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro- (9CI) (CA INDEX NAME)



RN 554430-73-8 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-ol, 8-[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro- (9CI) (CA INDEX NAME)

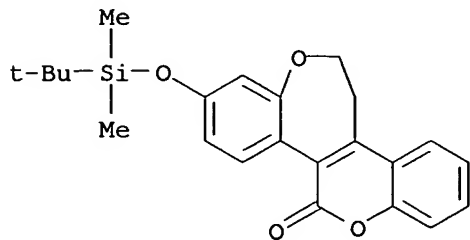




10/307,735

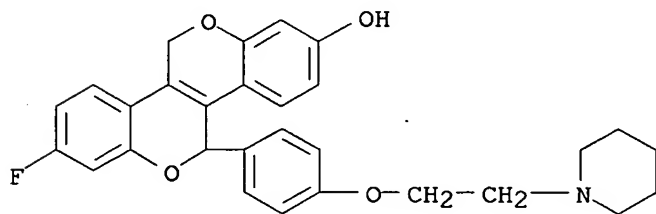
RN 554430-74-9 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 2-[[1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro- (9CI) (CA INDEX NAME)



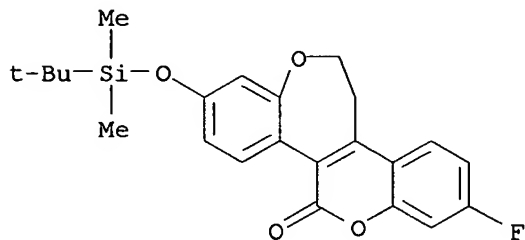
RN 554430-75-0 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2-ol, 8-fluoro-5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



RN 554430-77-2 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 2-[[1,1-dimethylethyl)dimethylsilyl]oxy]-8-fluoro-11,12-dihydro- (9CI) (CA INDEX NAME)



IT 554430-22-7P 554430-23-8P 554430-25-0P

554430-26-1P 554430-28-3P 554430-29-4P

554430-31-8P 554430-32-9P 554430-34-1P

554430-35-2P 554430-50-1P 554430-51-2P

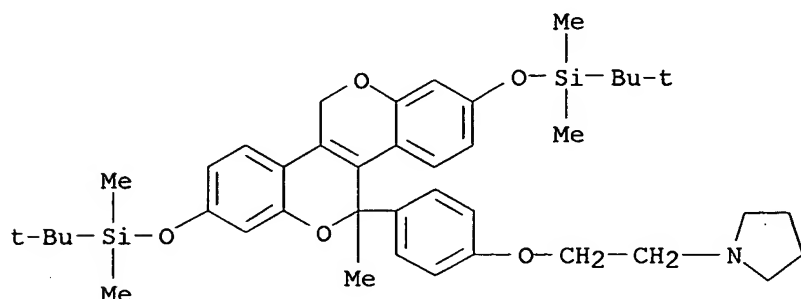
554430-52-3P 554431-90-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tetracyclic heterocycles as selective estrogen receptor modulators (SERMs))

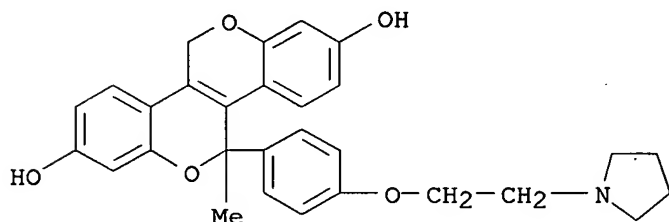
RN 554430-22-7 CAPLUS

CN Silane, [[5,11-dihydro-5-methyl-5-[4-[2-(1-pyrrolidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



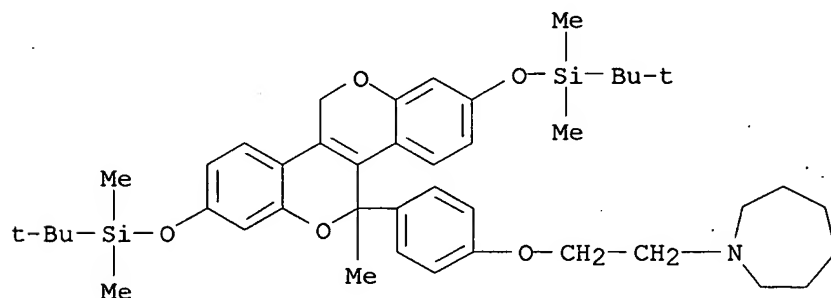
RN 554430-23-8 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-methyl-5-[4-[2-(1-pyrrolidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



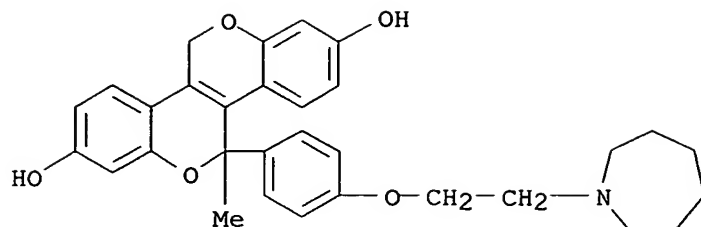
RN 554430-25-0 CAPLUS

CN Silane, [[5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-5,11-dihydro-5-methyl[1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



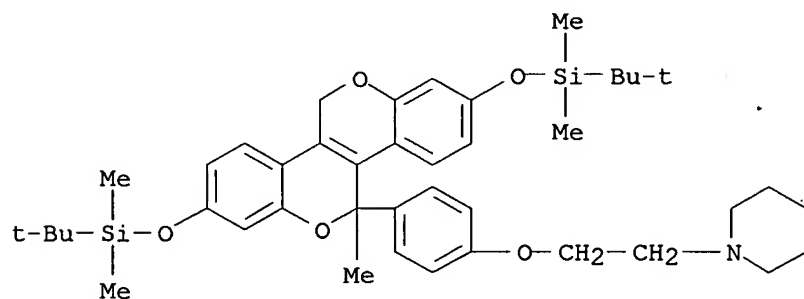
RN 554430-26-1 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-5,11-dihydro-5-methyl- (9CI) (CA INDEX NAME)



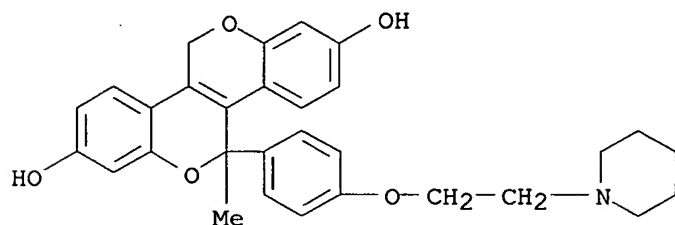
RN 554430-28-3 CAPLUS

CN Silane, [[5,11-dihydro-5-methyl-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



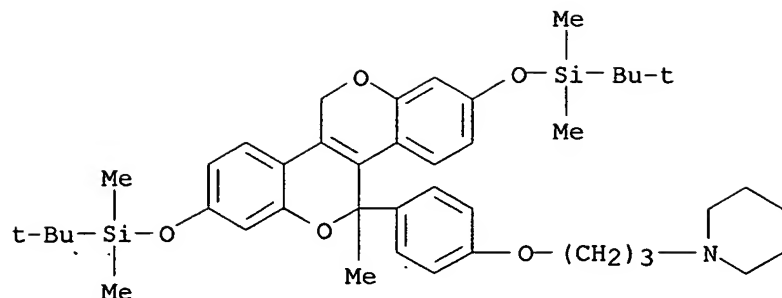
RN 554430-29-4 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-methyl-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



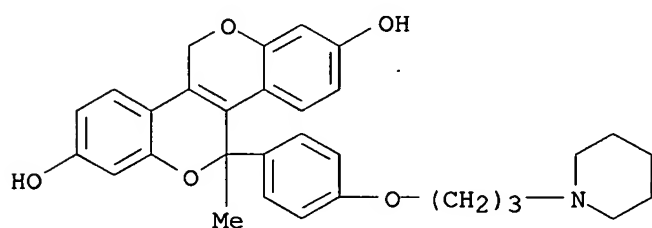
RN 554430-31-8 CAPLUS

CN Silane, [[5,11-dihydro-5-methyl-5-[4-[3-(1-piperidinyl)propoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



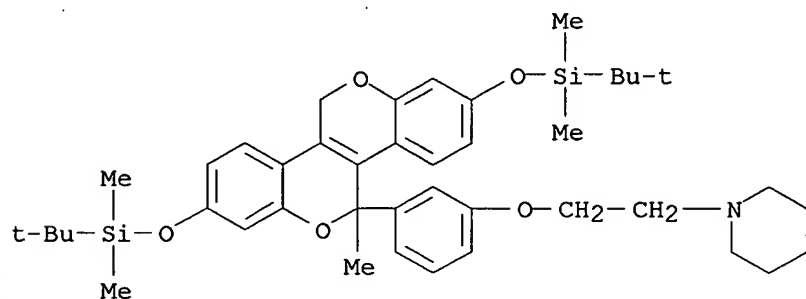
RN 554430-32-9 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-methyl-5-[4-[3-(1-piperidinyl)propoxy]phenyl]- (9CI) (CA INDEX NAME)



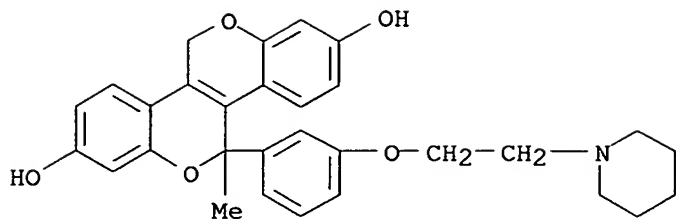
RN 554430-34-1 CAPLUS

CN Piperidine, 1-[2-[3-[2,8-bis[[1,1-dimethylethyl]dimethylsilyl]oxy]-5,11-dihydro-5-methyl[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



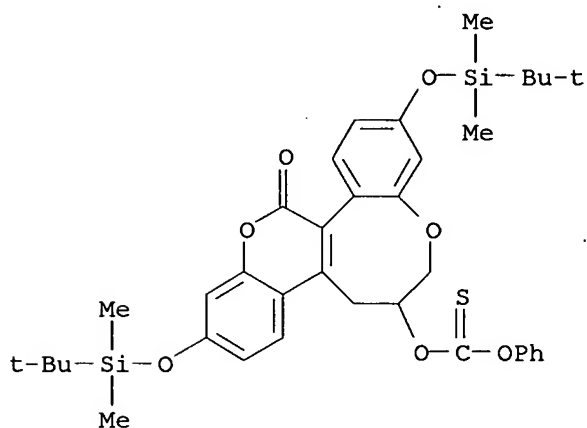
RN 554430-35-2 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-methyl-5-[3-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



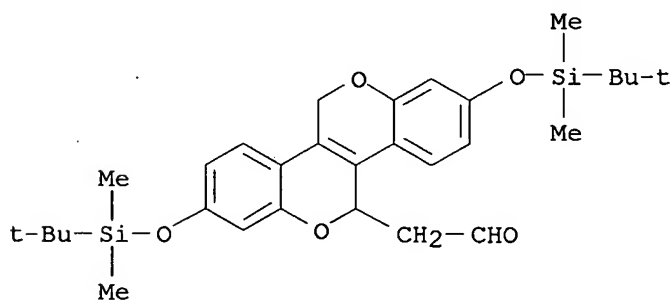
RN 554430-50-1 CAPLUS

CN Carbonothioic acid, O-[2,10-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,6,7,13-tetrahydro-13-oxo[1]benzopyrano[4,3-e][1]benzoxocin-6-yl] O-phenyl ester (9CI) (CA INDEX NAME)



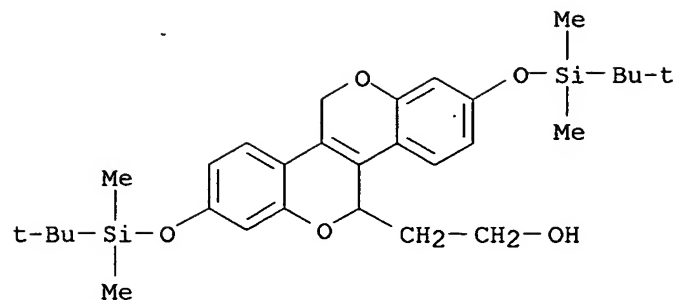
RN 554430-51-2 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5-acetaldehyde, 2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro- (9CI) (CA INDEX NAME)



RN 554430-52-3 CAPLUS

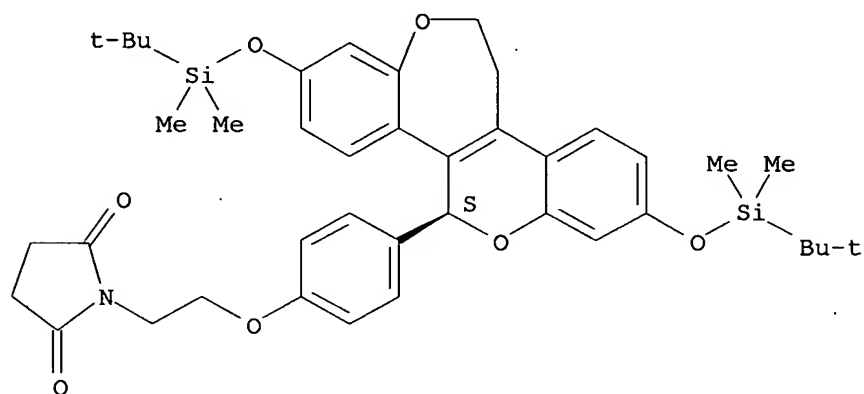
CN [1]Benzopyrano[4,3-c][1]benzopyran-5-ethanol, 2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro- (9CI) (CA INDEX NAME)



RN 554431-90-2 CAPLUS

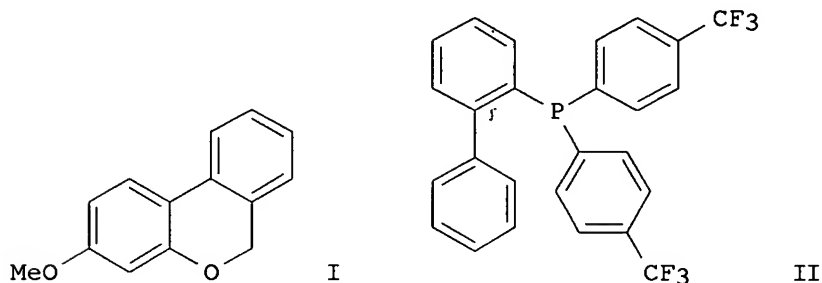
CN 2,5-Pyrrolidinedione, 1-[2-[4-[(5S)-2,8-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



122 ANSWER 2 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:553571 CAPLUS  
 DOCUMENT NUMBER: 141:140284  
 TITLE: Biaryl synthesis via direct arylation: establishment of an efficient catalyst for intramolecular processes  
 AUTHOR(S): Campeau, Louis-Charles; Parisien, Mathieu; Leblanc, Melissa; Fagnou, Keith  
 CORPORATE SOURCE: Center for Catalysis Research and Innovation, University of Ottawa, Ottawa, ON, K1N 6N5, Can.  
 SOURCE: Journal of the American Chemical Society (2004), 126(30), 9186-9187  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 141:140284  
 GI

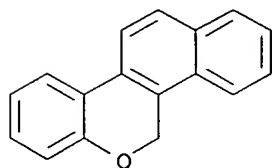


AB The direct arylation reaction with improved scope and catalyst activity for the intramol. formation of biaryl compds., e.g., I, is reported. This was achieved through the establishment of a highly active and robust catalyst system and the subsequent development of a phosphine ligand II. The enhanced catalytic activity, extended these transformations to include previously unreactive and poorly reactive substrates, and allowed for very low catalyst loadings.

IT **218-18-8P**, 5H-Benzo[b]naphtho[2,1-d]pyran  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of biaryls via palladium-catalyzed intramol. arylation of aryl bromophenylalkyl ethers, N-methyl-N-(phenyl)-bromobenzamide, and (bromophenylethyl)benzene in the presence of phosphine ligands)

RN 218-18-8 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran (8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~L22~~ ANSWER 3 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:548950 CAPLUS

DOCUMENT NUMBER: 141:134250

TITLE: Is it possible docking and scoring new ligands with few experimental data? Preliminary results on estrogen receptor as a case study

AUTHOR(S): Cozzini, P.; Dottorini, T.

CORPORATE SOURCE: Molecular Modelling Laboratory, Department of General and Inorganic Chemistry, Parco Area delle Scienze, University of Parma, Parma, 43100, Italy

SOURCE: European Journal of Medicinal Chemistry (2004), 39(7), 601-609

CODEN: EJMCA5; ISSN: 0223-5234

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Estrogens are steroid hormones playing critical roles in several physiol. processes, which bind the estrogen receptors ER $\alpha$  and ER $\beta$ . Aim of this work is to analyze, by different docking expts., the behavior of a set of compds., mimicking estrogens activity, to understand the relationship between ER $\alpha$  and such new ligands. Main goal is to verify, using a widely tested scoring software procedure applied on a set of 10 compds., the possibility to produce new lead candidate mols. in lack of, or with few exptl. data. The authors' preliminary results reveal the significance of HINT software as a scoring function in docking methodol. and specifically, as a mean for assessing the consistency of docking solns.

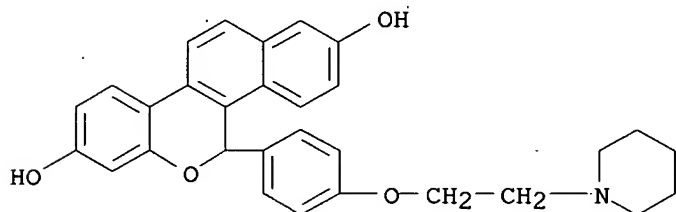
IT 188824-17-1

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(possible docking and scoring new ligands with few exptl. data in relation to preliminary results on estrogen receptor)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol, 5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



~~122~~ ANSWER 4 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:548891 CAPLUS

DOCUMENT NUMBER: 141:243297

TITLE: A facile synthesis of an unsymmetric  
benzopyranobenzopyran ring system

AUTHOR(S): Kanojia, Ramesh M.; Jain, Nareshkumar; Xu, Jiayi; Sui,  
Zhihua

CORPORATE SOURCE: Johnson & Johnson Pharmaceutical Research and  
Development, LLC, Raritan, NJ, 08869, USA

SOURCE: Tetrahedron Letters (2004), 45(30), 5837-5839  
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:243297

AB A facile route to the synthesis of an unsym. benzopyranobenzopyran ring  
system is described. A key feature of this synthesis incorporates a  
tandem deprotection-cyclization strategy to construct the C-ring of the  
tetracyclic system.

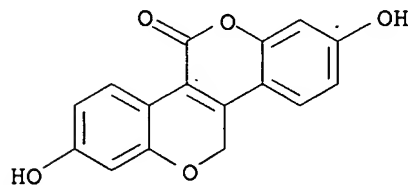
IT 554430-69-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis of an unsym. benzopyranobenzopyran ring system via tandem  
deprotection-cyclization strategy)

RN 554430-69-2 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5(11H)-one, 2,8-dihydroxy- (9CI) (CA  
INDEX NAME)



REFERENCE COUNT:

10

THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~122~~ ANSWER 5 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:42543 CAPLUS

DOCUMENT NUMBER: 140:246121

TITLE: Ligand-Based Structural Hypotheses for Virtual Screening

AUTHOR(S): Jain, Ajay N.

CORPORATE SOURCE: UCSF Cancer Research Institute and Comprehensive Cancer Center, University of California, San Francisco, CA, 94143-0128, USA

SOURCE: Journal of Medicinal Chemistry (2004), 47(4), 947-961  
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The majority of drug targets for small mol. therapeutics are proteins whose three-dimensional structure is not known to sufficient resolution to permit structure-based design. All three-dimensional QSAR approaches have a requirement for some hypothesis of ligand conformation and alignment, and predictions of mol. activity critically depend on this ligand-based binding site hypothesis. The mol. similarity function used in the Surflex docking system, coupled with quant. pressure to minimize overall mol. volume, forms an effective objective function for generating hypotheses of bioactive conformations of sets of small mols. binding to their cognate proteins. Results are presented, assessing utility of the method for ligands of the serotonin, histamine, muscarinic, and GABAA receptors. The Surflex similarity module (Surflex-Sim) was able, in each case, to distinguish true ligands from random compds. using models constructed from just two or three known ligands. True pos. rates of 60% were achieved with false pos. rates of 0-3%; the theor. enrichment rates were over 150-fold compared with random screening. The methods are practically applicable for rational design of ligands and for high-throughput virtual screening and offer competitive performance to many structure-based docking algorithms.

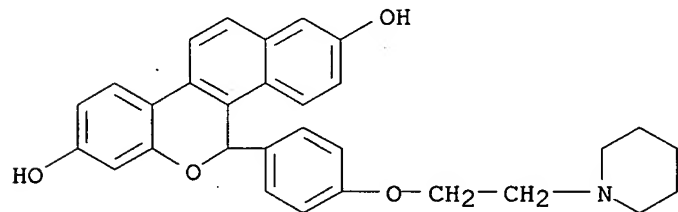
IT 188824-17-1, LY-357489

RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)

(estrogen receptor ligand; ligand-based structural hypotheses for virtual screening applied to ligands of different receptors and targets)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol, 5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

122 ANSWER 6 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:915312 CAPLUS

DOCUMENT NUMBER: 140:93958

TITLE: Carbon-carbon bond formation by radical cyclisation:  
Regioselective synthesis of coumarin-annulated sulfur  
heterocycles

AUTHOR(S): Majumdar, K. C.; Biswas, A.; Mukhopadhyay, P. P.

CORPORATE SOURCE: Department of Chemistry, University of Kalyani,  
Kalyani, 741 235, India

SOURCE: Synthesis (2003), (15), 2385-2389

CODEN: SYNTBF; ISSN: 0039-7881

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A simple convergent synthesis of cis-benzothiopyrano[3,2-c]benzopyran-7(2H)-ones (70-75%) through implementation of a regioselective 6-endo-trig aryl radical cyclization of the resp. 4-[(2-bromobenzyl)sulfanyl]-2H-chromen-2-ones (80-85%) with tributyltin hydride in the presence of a radical initiator (AIBN) is described. The starting materials are synthesized by phase-transfer-catalyzed reaction of 4-sulfanyl-2H-chromen-2-ones with 2-bromobenzyl bromides.

IT 645411-95-6P 645411-96-7P 645411-97-8P

645411-98-9P 645411-99-0P 645412-00-6P

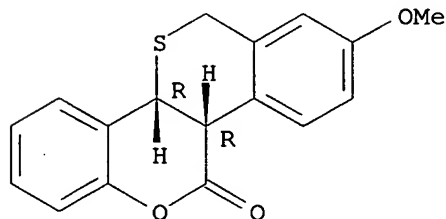
RL: SPN (Synthetic preparation); PREP (Preparation)

(carbon-carbon bond formation by radical cyclization and regioselective synthesis of coumarin-annulated sulfur heterocycles)

RN 645411-95-6 CAPLUS

CN 6H,11H-[2]Benzothiopyrano[4,3-c][1]benzopyran-11-one, 4b,10b-dihydro-8-methoxy-, (4bR,10bR)-rel- (9CI) (CA INDEX NAME)

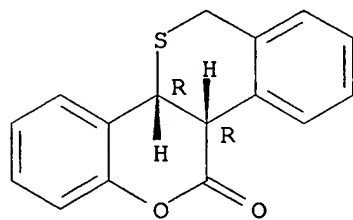
Relative stereochemistry.



RN 645411-96-7 CAPLUS

CN 6H,11H-[2]Benzothiopyrano[4,3-c][1]benzopyran-11-one, 4b,10b-dihydro-, (4bR,10bR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

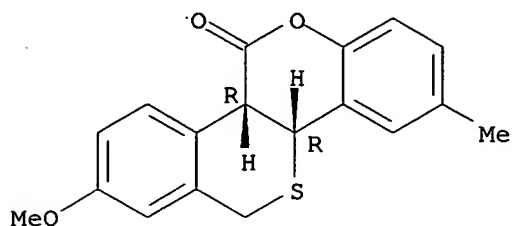


10/307,735

RN 645411-97-8 CAPLUS

CN 6H,11H-[2]Benzothiopyrano[4,3-c][1]benzopyran-11-one, 4b,10b-dihydro-8-methoxy-3-methyl-, (4bR,10bR)-rel- (9CI) (CA INDEX NAME)

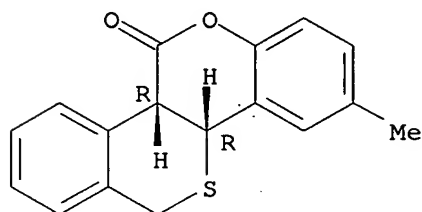
Relative stereochemistry.



RN 645411-98-9 CAPLUS

CN 6H,11H-[2]Benzothiopyrano[4,3-c][1]benzopyran-11-one, 4b,10b-dihydro-3-methyl-, (4bR,10bR)-rel- (9CI) (CA INDEX NAME)

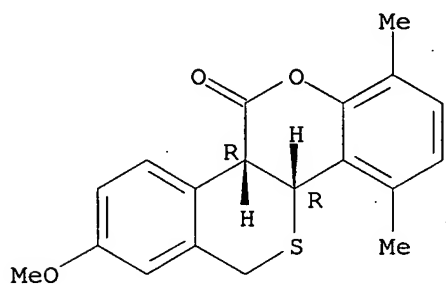
Relative stereochemistry.



RN 645411-99-0 CAPLUS

CN 6H,11H-[2]Benzothiopyrano[4,3-c][1]benzopyran-11-one, 4b,10b-dihydro-8-methoxy-1,4-dimethyl-, (4bR,10bR)-rel- (9CI) (CA INDEX NAME)

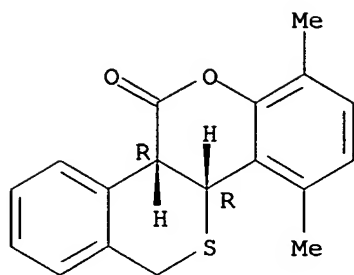
Relative stereochemistry.



RN 645412-00-6 CAPLUS

CN 6H,11H-[2]Benzothiopyrano[4,3-c][1]benzopyran-11-one, 4b,10b-dihydro-1,4-dimethyl-, (4bR,10bR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT:

46

THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/307,735

~~L2~~ ANSWER 7 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:807792 CAPLUS

DOCUMENT NUMBER: 140:391166

TITLE: Product class 4: benzopyranones and benzopyranthiones

AUTHOR(S): Williams, A. C.; Camp, N.

CORPORATE SOURCE: Germany

SOURCE: Science of Synthesis (2003), 14, 347-638

CODEN: SSCYJ9

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review. Methods for preparing 2H-1-benzopyran-2-ones, 4H-1-benzopyran-4-ones, 1H-2-benzopyran-1-ones, 6H-dibenzo[b,d]pyran-6-ones, 9H-xanthenones and their corresponding thione analogs as well as 3H-2-benzopyran-3-ones are surveyed. Synthetic methods include ring closure, ring transformation, aromatization and substituent modification reactions.

IT 13225-81-5P 20503-15-5P 80360-50-5P

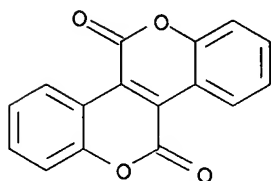
80360-51-6P 80360-52-7P 685828-95-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(review of preparation of benzopyranones and benzopyranthiones via ring closure, ring transformations, aromatization and substituent modifications)

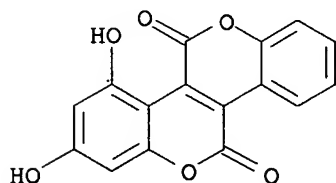
RN 13225-81-5 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione (8CI, 9CI) (CA INDEX NAME)



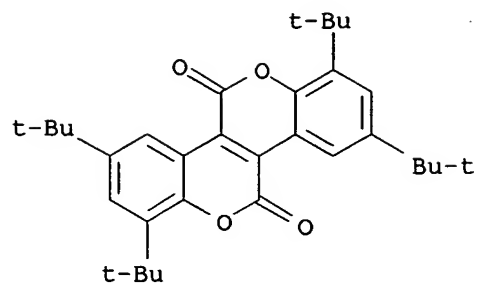
RN 20503-15-5 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 2,4-dihydroxy- (8CI, 9CI)  
(CA INDEX NAME)



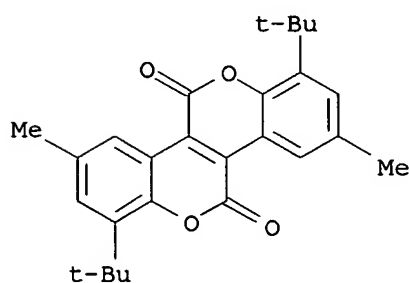
RN 80360-50-5 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 1,3,7,9-tetrakis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



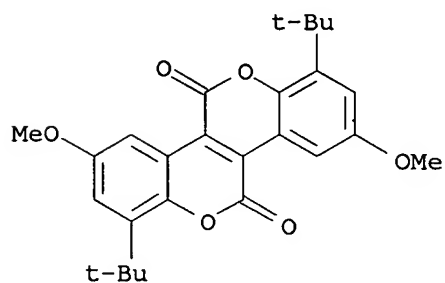
RN 80360-51-6 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 1,7-bis(1,1-dimethylethyl)-3,9-dimethyl- (9CI) (CA INDEX NAME)



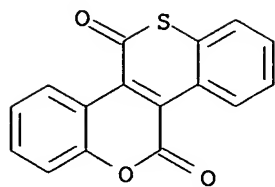
RN 80360-52-7 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 1,7-bis(1,1-dimethylethyl)-3,9-dimethoxy- (9CI) (CA INDEX NAME)



RN 685828-95-9 CAPLUS

CN [1]Benzothiopyrano[4,3-c][1]benzopyran-5,11-dione (9CI) (CA INDEX NAME)



REFERENCE COUNT:

1083 THERE ARE 1083 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT



122 ANSWER 8 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:758920 CAPLUS

DOCUMENT NUMBER: 139:395590

TITLE: Photoreactions of 3-Diazo-3H-benzofuran-2-one;

Dimerization and Hydrolysis of Its Primary

Photoproduct, A Quinonoid Cumulenone: A Study by

Time-Resolved Optical and Infrared Spectroscopy

AUTHOR(S): Chiang, Yvonne; Gaplovsky, Martin; Kresge, A. Jerry;  
Leung, King Hung; Ley, Christian; Mac, Marek; Persy,  
Gabriele; Phillips, David L.; Popik, Vladimir V.;

Roedig, Christoph; Wirz, Jakob; Zhu, Yu

CORPORATE SOURCE: The Department of Chemistry, University of Toronto,  
Toronto, ON, M5S 3H6, Can.

SOURCE: Journal of the American Chemical Society (2003),  
125(42), 12872-12880

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:395590

AB Light-induced deazotization of 3-diazo-3H-benzofuran-2-one (1) in solution is accompanied by facile (CO)-O bond cleavage yielding 6-(oxoethenylidene)-2,4-cyclohexadien-1-one (3), which appears with a rise time of 28 ps. The expected Wolff-rearrangement product, 7-oxabicyclo[4.2.0]octa-1,3,5-trien-8-ylidenemethanone (4), is not formed. The efficient light-induced formation of the quinonoid cumulenone 3 opens the way to determine the reactivity of a cumulenone in solution. The reaction kinetics of 3 were monitored by nanosecond flash photolysis with optical ( $\lambda_{\text{max}} \approx 460$  nm) as well as Raman (1526  $\text{cm}^{-1}$ ) and IR detection (2050  $\text{cm}^{-1}$ ). Remarkably, the reactivity of 3 is that expected from its valence isomer, the cyclic carbene 3H-benzofuran-2-one-3-ylidene, 2. In aqueous solution, acid-catalyzed addition of water forms the lactone 3-hydroxy-3H-benzofuran-2-one (5). The reaction is initiated by protonation of the cumulenone on its  $\beta$ -carbon atom. In hexane, cumulenone 3 dimerizes to isoxindigo ((E)-[3,3']bibenzofuranylidene-2,2'-dione, 7), coumestan (6H-benzofuro[3,2-c][1]benzopyran-6-one, 8), and a small amount of dibenzonaphthyrone ([1]benzopyrano[4,3-][1]benzopyran-5,11-dione, 9) at a nearly diffusion-controlled rate. Ab initio calcns. (G3) are consistent with the observed data. Carbene 2 is predicted to have a singlet ground state, which undergoes very facile, strongly exothermic (irreversible) ring opening to the cumulenone 3. The calculated barrier to formation of 4 (Wolff-rearrangement) is prohibitive. DFT calcns. indicate that protonation of 3 on the  $\beta$ -carbon is accompanied by cyclization to the protonated carbene  $2\text{H}^+$ , and that dimerization of 3 to 7 and 9 takes place in a single step with negligible activation energy.

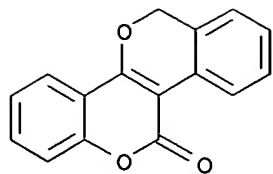
IT 96600-94-1P

RL: BYP (Byproduct); PREP (Preparation)

(photoreactions of diazobenzofuranone dimerization and hydrolysis of its primary photoproduct)

RN 96600-94-1 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-11-one (9CI) (CA INDEX NAME)



REFERENCE COUNT:

44

THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

22 ANSWER 9 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:678670 CAPLUS

DOCUMENT NUMBER: 139:192008

TITLE: Methods and composition for treating decreased libido in women with estrogenic components

INVENTOR(S): Coelingh Bennink, Herman Jian Tijmen

PATENT ASSIGNEE(S): Pantarhei Bioscience B.V., Neth.

SOURCE: PCT Int. Appl., 17 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003070253	A1	20030828	WO 2003-NL125	20030219
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.:

EP 2002-75696

A 20020221

AB The present invention is concerned with a method of treating decreased libido in pre-menopausal women, said decreased libido being the result of the repeated administration of a progestogenic component, wherein the method comprises the administration of the estrogenic component to a woman in an effective amount to improve the woman's libido. The present method is particularly suited for treating decreased libido in women using hormonal contraceptives that employ administration of a progestogenic component.

IT 188824-17-1, LY-357489

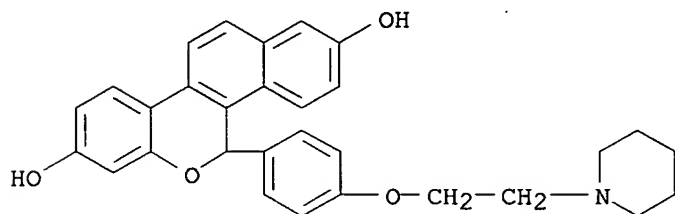
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)

(methods and composition for treating decreased libido in women with estrogenic components)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol, 5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

9

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 10 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:511339 CAPLUS

DOCUMENT NUMBER: 139:85328

TITLE: Preparation of tetracyclic heterocycles as selective estrogen receptor modulators (SERMs).

INVENTOR(S): Kanojia, Ramesh M.; Jain, Nareshkumar F.; Ng, Raymond; Sui, Zhihua; Xu, Jiayi

PATENT ASSIGNEE(S): Ortho-McNeil Pharmaceutical, Inc., USA

SOURCE: PCT Int. Appl., 306 pp.

CODEN: PIXXD2

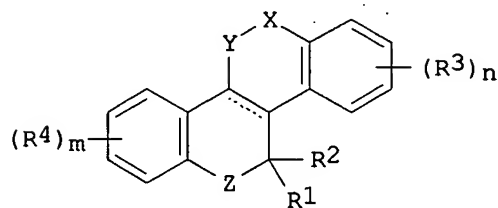
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003053977	A1	20030703	WO 2002-US38486	20021202
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
BR 2002015152	A	20041019	BR 2002-15152	20021202
EP 1467998	A1	20041020	EP 2002-797167	20021202
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK			
PRIORITY APPLN. INFO.:			US 2001-341957P	P 20011219
			WO 2002-US38486	W 20021202
OTHER SOURCE(S):	MARPAT 139:85328			
GI				



AB Title compds. [I; dotted line = optional double bond; X = O, S, CRaRb, CO; Y = CRaRb, CRaRb(CRaRb)1-2, CRaRbCO, CRaRbCOCRaRb, CO, O, S; Z = O, S; R1 = H, (substituted) alkyl, alkenyl, cycloalkyl, aryl, aroyl, aralkyl, heteroaryl, heteroarylalkyl; R2 = OH, (substituted) alkyl, alkenyl, cycloalkyl, aryl, aroyl, aralkyl, heteroaryl, heteroarylalkyl; R1R2 = O; m, n = 0-4; R3, R4 = halo, OH, amino, NO2, cyano, CORg, CO2Rg, etc.; Rg = H, alkyl, aryl, aralkyl, 1,7,7-trimethyl-2-oxabicyclo[2.2.1]heptan-3-one; with provisos], were prepared Thus, 3-(2-hydroxy-4-methoxyphenyl)-7-hydroxy-

4-methylchromen-2-one (preparation given), in methanol/acetone was added at room temperature anhydrous potassium carbonate; the solution was stirred 2 h to give

2,8-dihydroxy-1H-chromeno[4,3-c]chromen-5-one. The latter bound to estrogen  $\alpha$  and  $\beta$  receptors at 0.505  $\mu\text{M}$  and 0.061  $\mu\text{M}$ , resp. I are useful in the treatment and/or prevention of disorders associated with the depletion of estrogen such as hot flashes, vaginal dryness, osteopenia and osteoporosis; hormone sensitive cancers and hyperplasia of the breast, endometrium, cervix and prostate; endometriosis, uterine fibroids, osteoarthritis and as contraceptive agents, alone or in combination with a progestogen or progestogen antagonist.

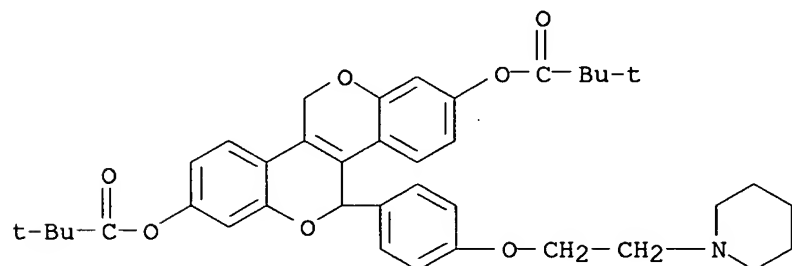
IT 554429-87-7P 554429-88-8P 554429-89-9P  
554429-90-2P 554429-91-3P 554429-92-4P  
554429-93-5P 554429-94-6P 554429-95-7P  
554429-96-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of tetracyclic heterocycles as selective estrogen receptor modulators (SERMs))

RN 554429-87-7 CAPLUS

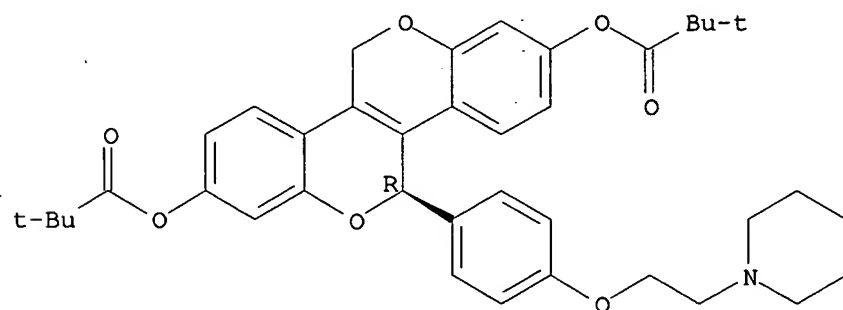
CN Propanoic acid, 2,2-dimethyl-, 5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl ester (9CI) (CA INDEX NAME)



RN 554429-88-8 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, (5R)-5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl ester (9CI) (CA INDEX NAME)

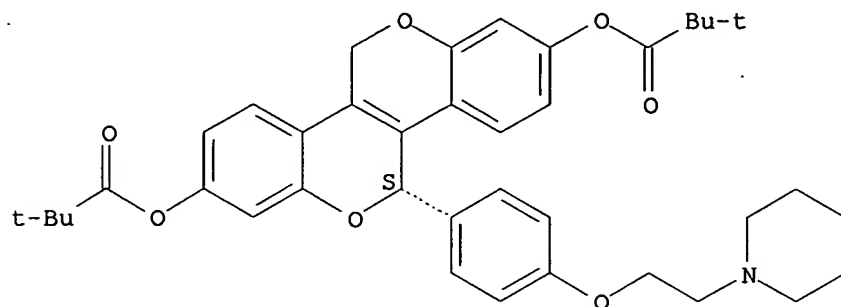
Absolute stereochemistry.



RN 554429-89-9 CAPLUS

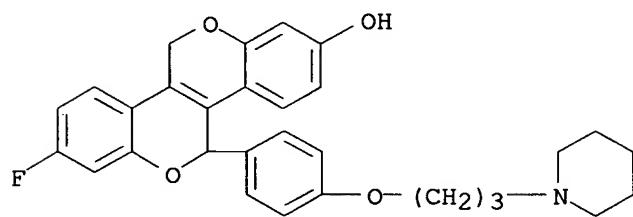
CN Propanoic acid, 2,2-dimethyl-, (5S)-5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



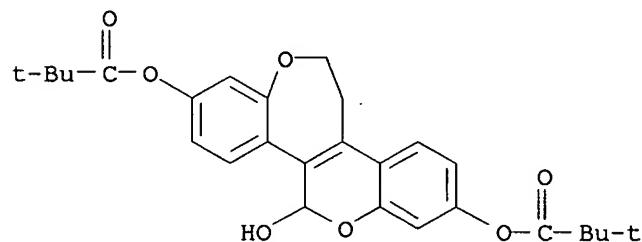
RN 554429-90-2 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2-ol, 8-fluoro-5,11-dihydro-5-[4-[3-(1-piperidinyl)propoxy]phenyl]- (9CI) (CA INDEX NAME)



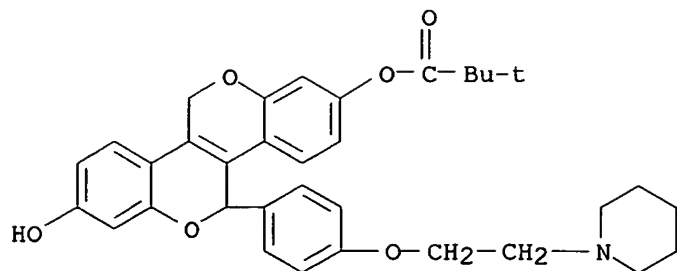
RN 554429-91-3 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 11,12-dihydro-5-hydroxy-5H-[1]benzopyrano[4,3-d][1]benzoxepin-2,8-diyl ester (9CI) (CA INDEX NAME)



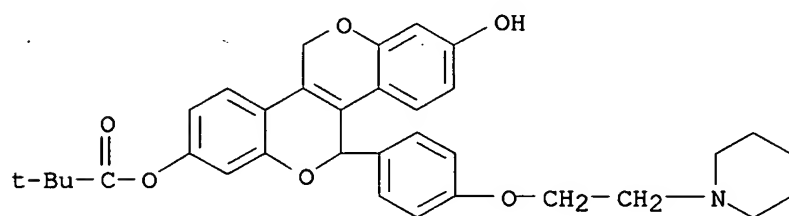
RN 554429-92-4 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 5,11-dihydro-8-hydroxy-5-[4-[3-(1-piperidinyl)propoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2-yl ester (9CI) (CA INDEX NAME)



RN 554429-93-5 CAPLUS

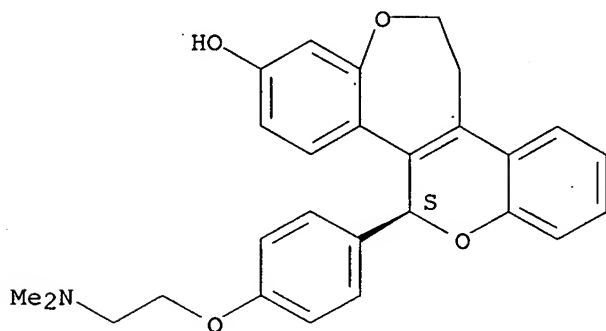
CN Propanoic acid, 2,2-dimethyl-, 5,11-dihydro-8-hydroxy-11-[4-[2-(1-piperidinyl)ethoxy]phenyl]-[1]benzopyrano[4,3-c][1]benzopyran-2-yl ester (9CI) (CA INDEX NAME)



RN 554429-94-6 CAPLUS

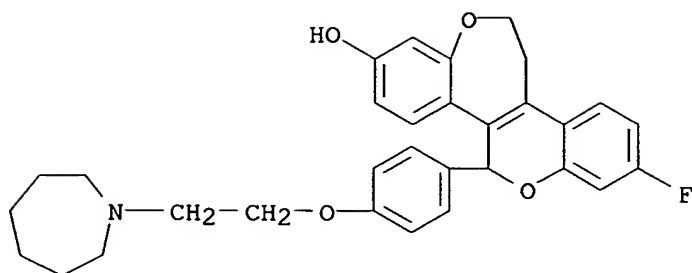
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 5-[4-[2-(dimethylamino)ethoxy]phenyl]-11,12-dihydro-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 554429-95-7 CAPLUS

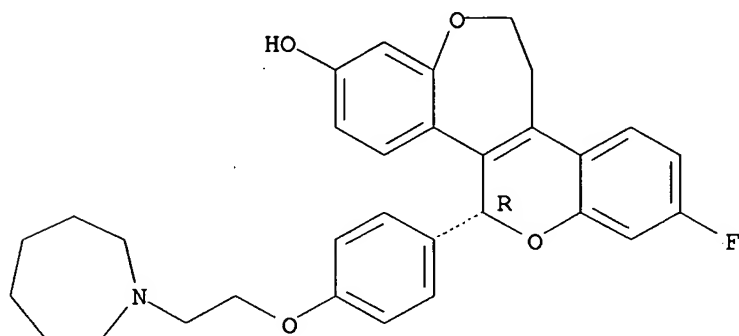
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 8-fluoro-5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro- (9CI) (CA INDEX NAME)



RN 554429-96-8 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 8-fluoro-5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro-, (5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 554429-97-9P 554430-39-6P 554430-43-2P  
 554430-44-3P 554430-45-4P 554430-48-7P  
 554430-60-3P 554430-85-2P 554430-86-3P  
 554430-87-4P 554430-88-5P 554430-89-6P  
 554430-90-9P 554430-91-0P 554430-92-1P  
 554430-93-2P 554430-94-3P 554430-95-4P  
 554430-96-5P 554430-97-6P 554430-98-7P  
 554430-99-8P 554431-00-4P 554431-01-5P  
 554431-02-6P 554431-03-7P 554431-04-8P  
 554431-05-9P 554431-06-0P 554431-07-1P  
 554431-08-2P 554431-09-3P 554431-10-6P  
 554431-11-7P 554431-12-8P 554431-13-9P  
 554431-14-0P 554431-15-1P 554431-16-2P  
 554431-17-3P 554431-18-4P 554431-19-5P  
 554431-20-8P 554431-21-9P 554431-22-0P  
 554431-23-1P 554431-24-2P 554431-25-3P  
 554431-26-4P 554431-27-5P 554431-28-6P  
 554431-29-7P 554431-30-0P 554431-31-1P  
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 554431-35-5P 554431-36-6P 554431-37-7P  
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 554431-83-3P 554431-84-4P 554431-85-5P  
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 554433-06-6P

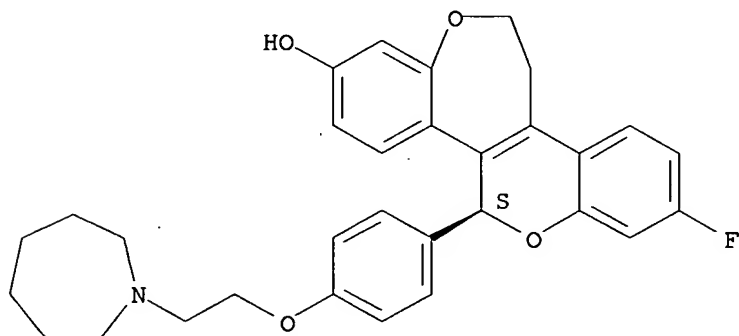
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of tetracyclic heterocycles as selective estrogen receptor modulators (SERMs))

RN 554429-97-9 CAPLUS

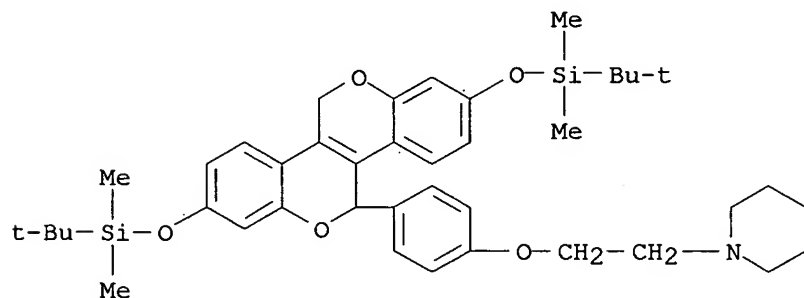
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 8-fluoro-5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



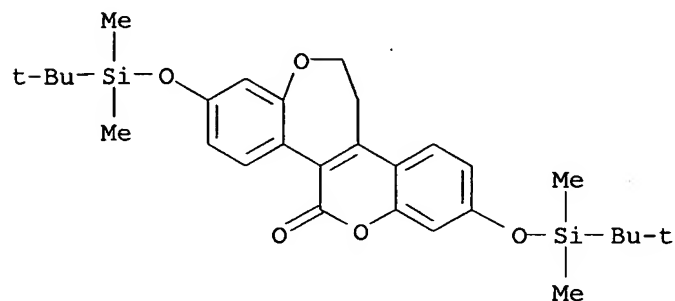
RN 554430-39-6 CAPLUS

CN Silane, [[5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



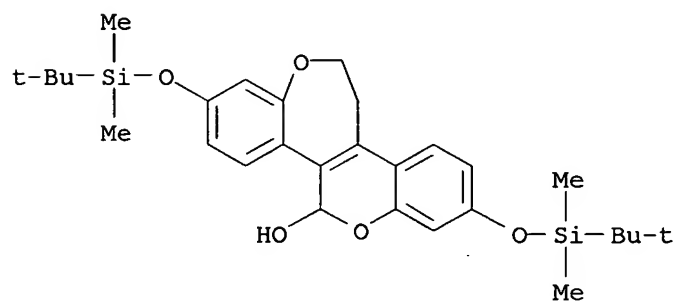
RN 554430-43-2 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro- (9CI) (CA INDEX NAME)



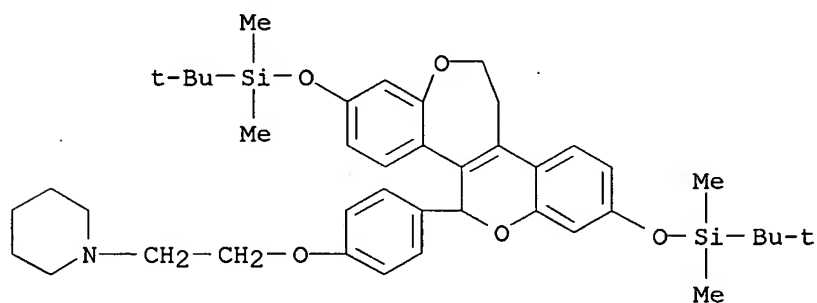
RN 554430-44-3 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-ol, 2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro- (9CI) (CA INDEX NAME)



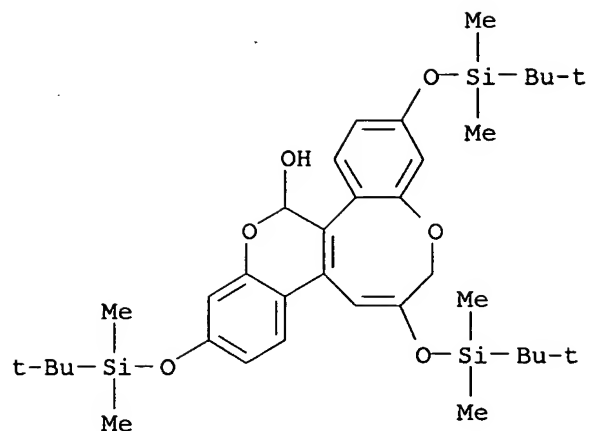
RN 554430-45-4 CAPLUS

CN Piperidine, 1-[2-[4-[2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



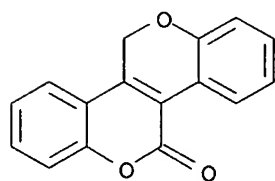
RN 554430-48-7 CAPLUS

CN [1]Benzopyrano[4,3-e][1]benzoxocin-13-ol, 2,6,10-tris[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7,13-dihydro- (9CI) (CA INDEX NAME)



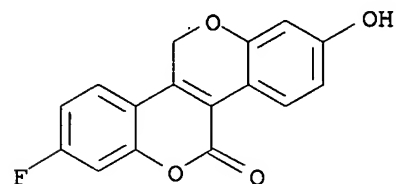
RN 554430-60-3 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5(11H)-one (9CI) (CA INDEX NAME)



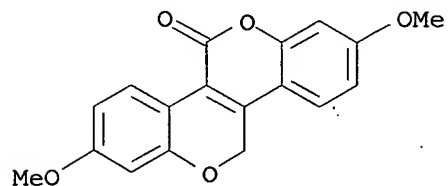
RN 554430-85-2 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5(11H)-one, 8-fluoro-2-hydroxy- (9CI)  
(CA INDEX NAME)



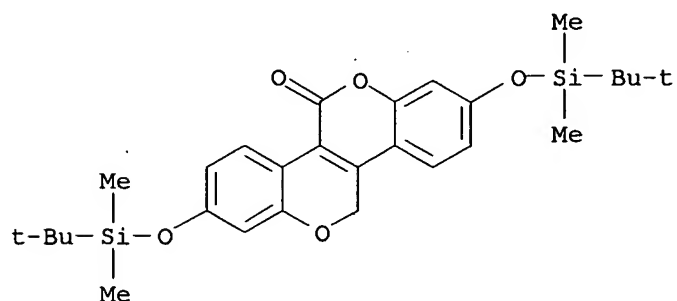
RN 554430-86-3 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5(11H)-one, 2,8-dimethoxy- (9CI) (CA INDEX NAME)



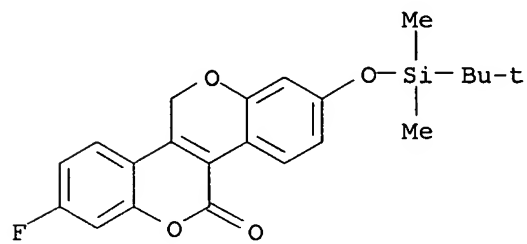
RN 554430-87-4 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5(11H)-one, 2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]- (9CI) (CA INDEX NAME)



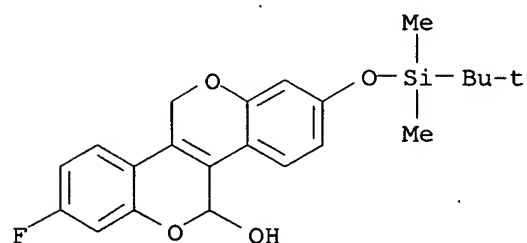
RN 554430-88-5 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5(11H)-one, 2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-fluoro- (9CI) (CA INDEX NAME)



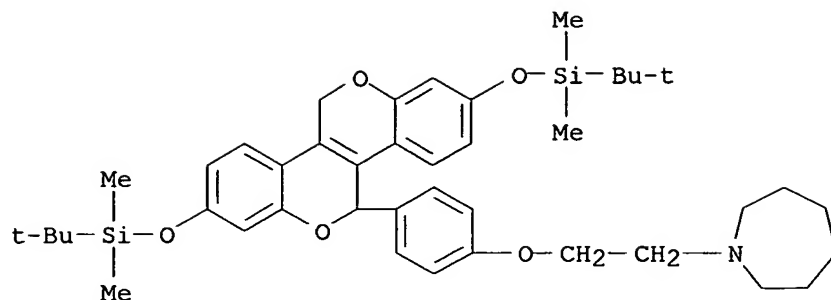
RN 554430-89-6 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5-ol, 2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-fluoro-5,11-dihydro- (9CI) (CA INDEX NAME)



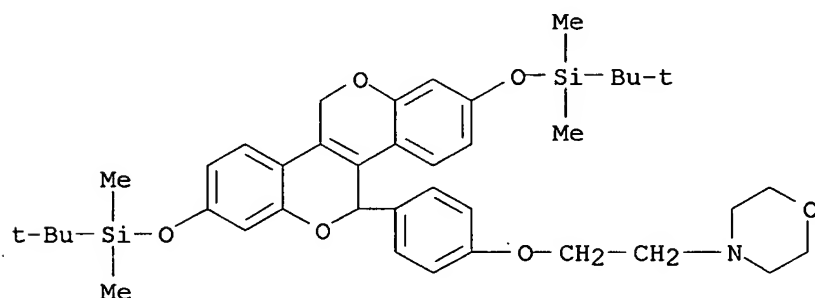
RN 554430-90-9 CAPLUS

CN 1H-Azepine, 1-[2-[4-[2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]hexahydro- (9CI) (CA INDEX NAME)



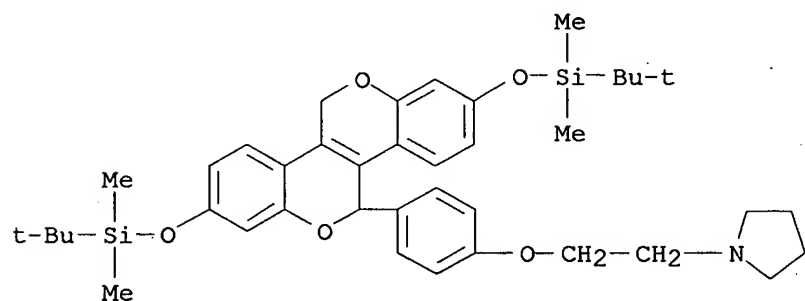
RN 554430-91-0 CAPLUS

CN Morpholine, 4-[2-[4-[2,8-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



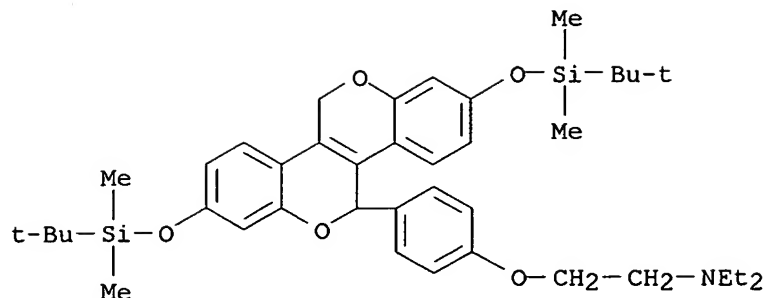
RN 554430-92-1 CAPLUS

CN Pyrrolidine, 1-[2-[4-[2,8-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



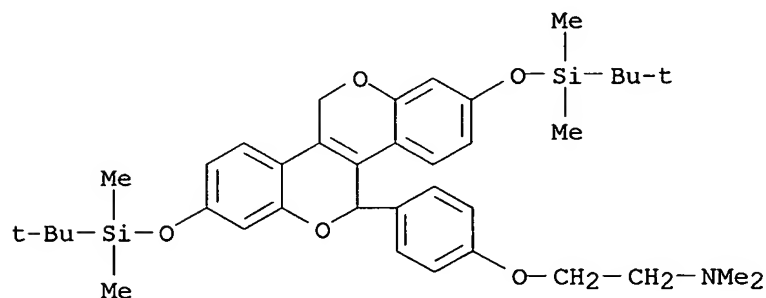
RN 554430-93-2 CAPLUS

CN Ethanamine, 2-[4-[2,8-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]-N,N-diethyl- (9CI) (CA INDEX NAME)



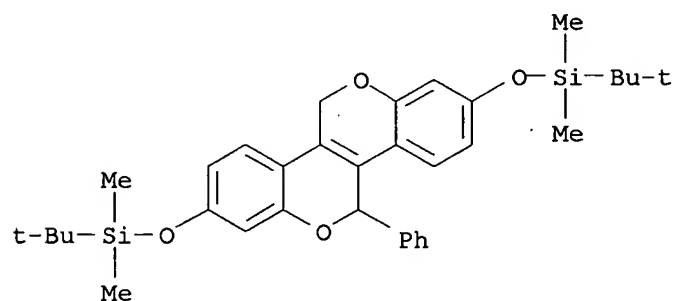
RN 554430-94-3 CAPLUS

CN Ethanamine, 2-[4-[2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]-N,N-dimethyl- (9CI) (CA INDEX NAME)



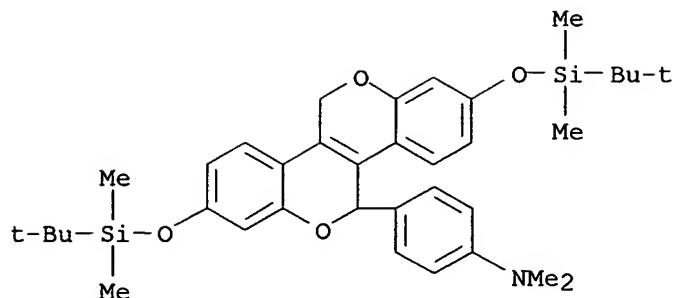
RN 554430-95-4 CAPLUS

CN Silane, [(5,11-dihydro-5-phenyl[1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl)bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



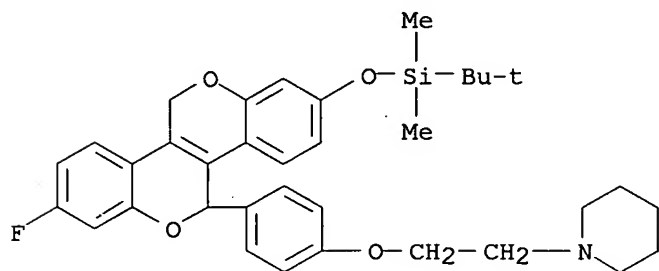
RN 554430-96-5 CAPLUS

CN Benzenamine, 4-[2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



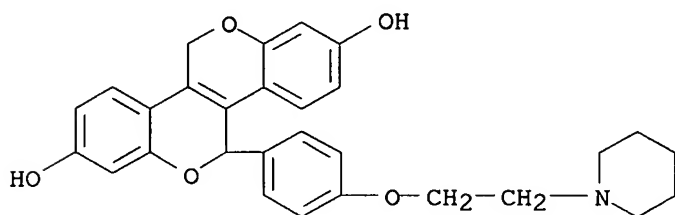
RN 554430-97-6 CAPLUS

CN Piperidine, 1-[2-[4-[2-bis[[[1,1-dimethylethyl]dimethylsilyl]oxy]-8-fluoro-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]- (9CI)  
(CA INDEX NAME)



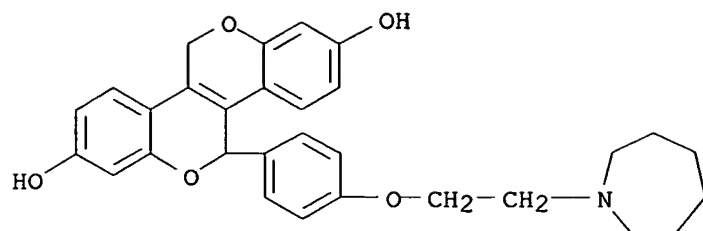
RN 554430-98-7 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



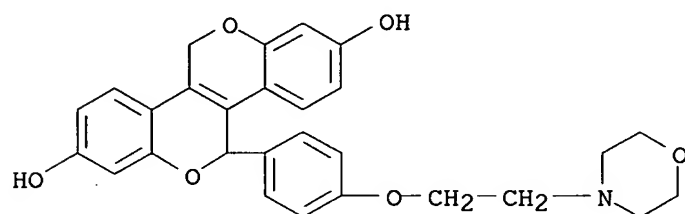
RN 554430-99-8 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-5,11-dihydro- (9CI) (CA INDEX NAME)



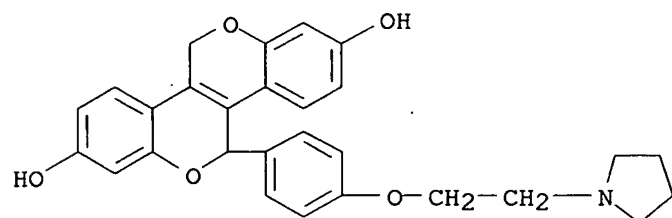
RN 554431-00-4 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-[4-[2-(4-morpholinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



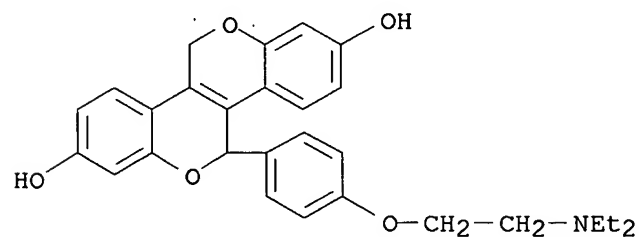
RN 554431-01-5 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-[4-[2-(1-pyrrolidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



RN 554431-02-6 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5-[4-[2-(diethylamino)ethoxy]phenyl]-5,11-dihydro- (9CI) (CA INDEX NAME)

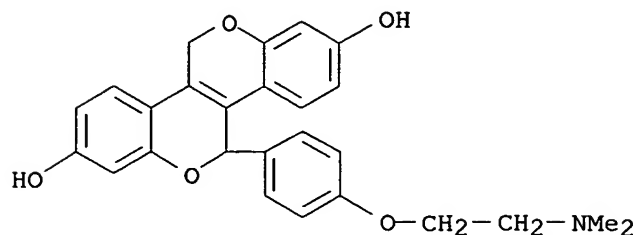


RN 554431-03-7 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5-[4-[2-

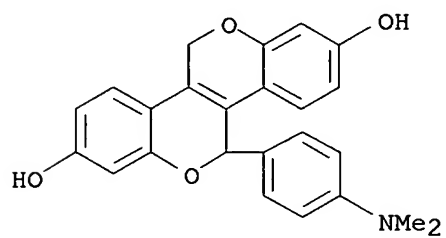


(dimethylamino)ethoxy]phenyl]-5,11-dihydro- (9CI) (CA INDEX NAME)



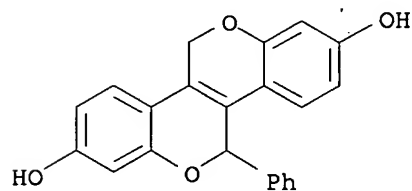
RN 554431-04-8 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5-[4-(dimethylamino)phenyl]-5,11-dihydro- (9CI) (CA INDEX NAME)



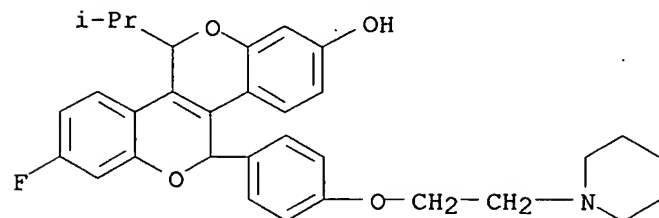
RN 554431-05-9 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-phenyl- (9CI) (CA INDEX NAME)



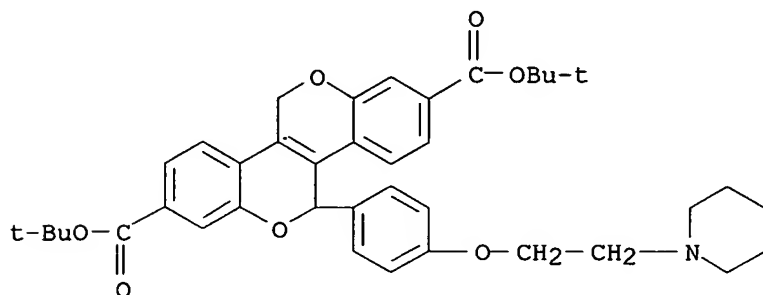
RN 554431-06-0 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2-ol, 8-fluoro-5,11-dihydro-11-(1-methylethyl)-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



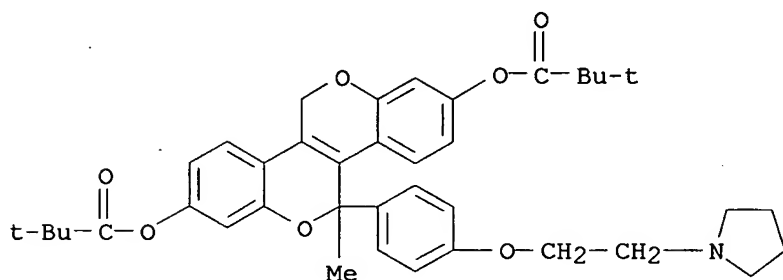
RN 554431-07-1 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-dicarboxylic acid,  
5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, bis(1,1-  
dimethylethyl) ester (9CI) (CA INDEX NAME)



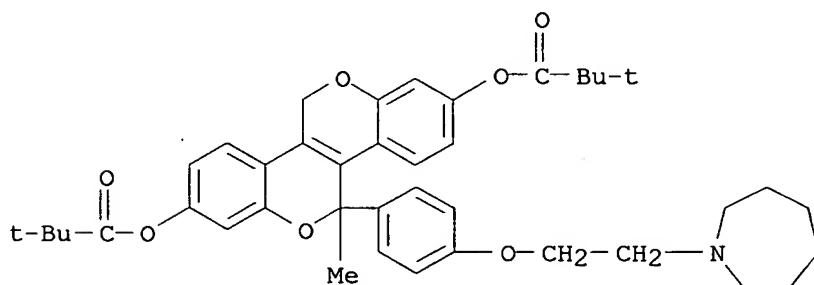
RN 554431-08-2 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 5,11-dihydro-5-methyl-5-[4-[2-(1-pyrrolidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl ester (9CI) (CA INDEX NAME)



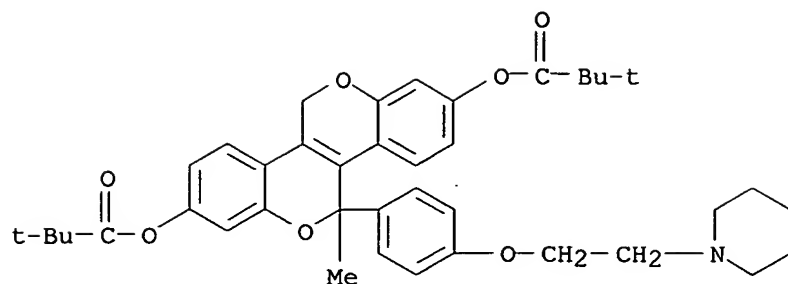
RN 554431-09-3 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-5,11-dihydro-5-methyl[1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl ester (9CI) (CA INDEX NAME)



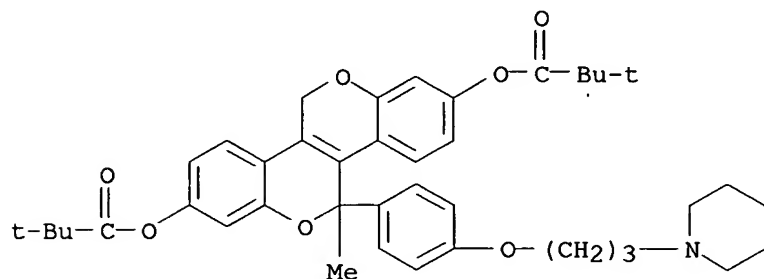
RN 554431-10-6 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 5,11-dihydro-5-methyl-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl ester (9CI) (CA INDEX NAME)



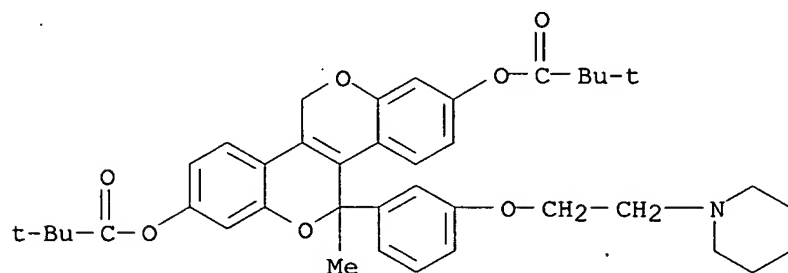
RN 554431-11-7 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 5,11-dihydro-5-methyl-5-[4-[3-(1-piperidinyl)propoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl ester (9CI) (CA INDEX NAME)



RN 554431-12-8 CAPLUS

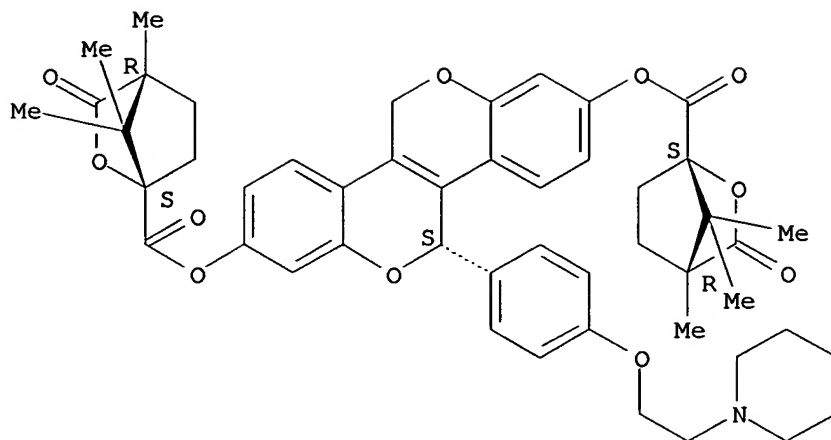
CN Propanoic acid, 2,2-dimethyl-, 5,11-dihydro-5-methyl-5-[3-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl ester (9CI) (CA INDEX NAME)



RN 554431-13-9 CAPLUS

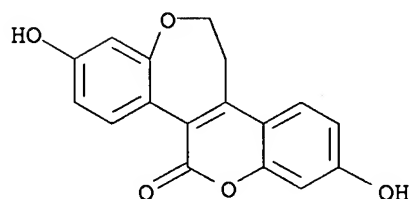
CN 2-Oxabicyclo[2.2.1]heptane-1-carboxylic acid, 4,7,7-trimethyl-3-oxo-, (5S)-5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl ester, (1S,1'S,4R,4'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



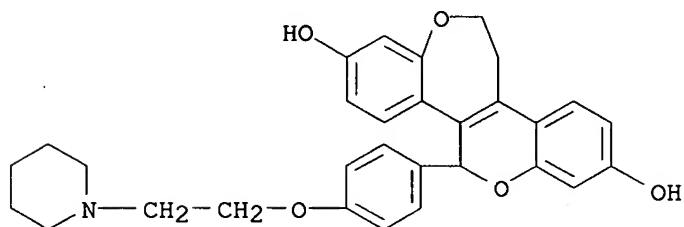
RN 554431-14-0 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 11,12-dihydro-2,8-dihydroxy-  
(9CI) (CA INDEX NAME)



RN 554431-15-1 CAPLUS

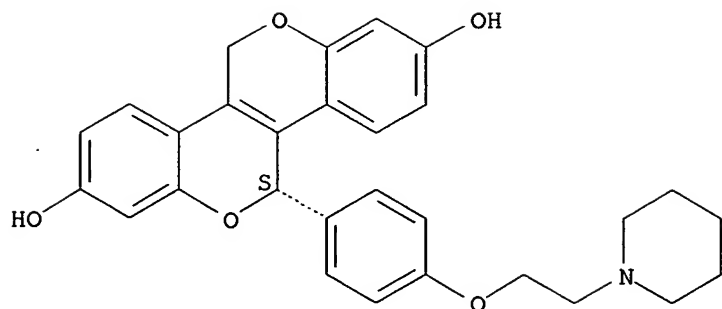
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 11,12-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



RN 554431-16-2 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (5S)- (9CI) (CA INDEX NAME)

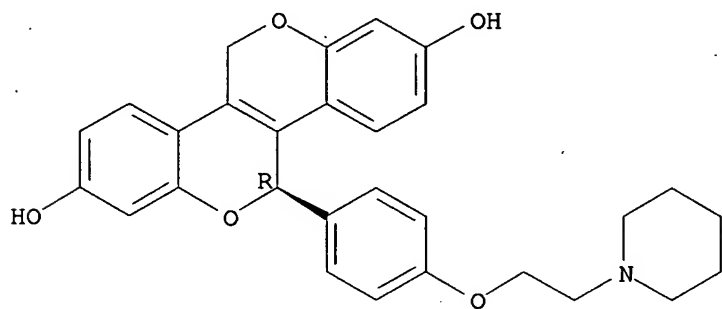
Absolute stereochemistry. Rotation (-).



RN 554431-17-3 CAPLUS

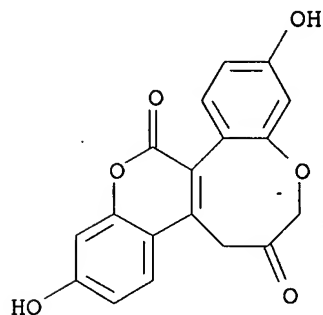
CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



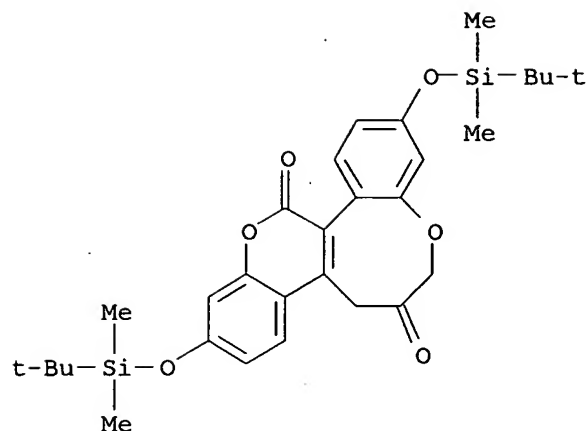
RN 554431-18-4 CAPLUS

CN [1]Benzopyrano[4,3-e][1]benzoxocin-6,13(5H,7H)-dione, 2,10-dihydroxy-, (9CI) (CA INDEX NAME)



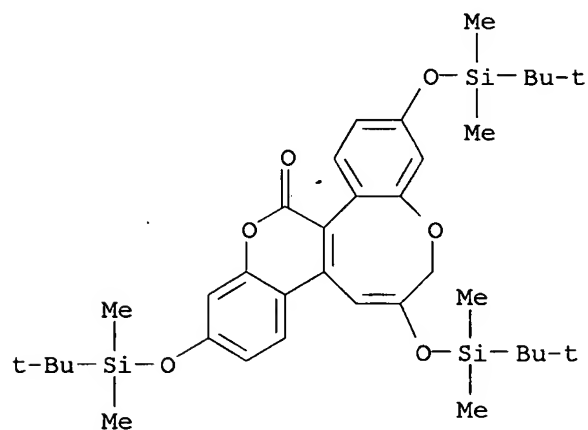
RN 554431-19-5 CAPLUS

CN [1]Benzopyrano[4,3-e][1]benzoxocin-6,13(5H,7H)-dione, 2,10-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]- (9CI) (CA INDEX NAME)



RN 554431-20-8 CAPLUS

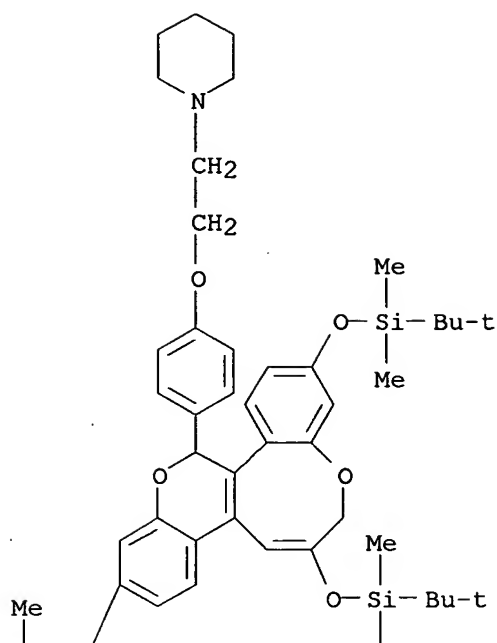
CN [1]Benzopyrano[4,3-e][1]benzoxocin-13(7H)-one, 2,6,10-tris[[1,1-dimethylethyl)dimethylsilyl]oxy]- (9CI) (CA INDEX NAME)



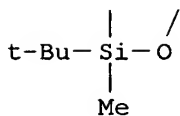
RN 554431-21-9 CAPLUS

CN Piperidine, 1-[2-[4-[2,6,10-tris[[1,1-dimethylethyl)dimethylsilyl]oxy]-7,13-dihydro[1]benzopyrano[4,3-e][1]benzoxocin-13-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

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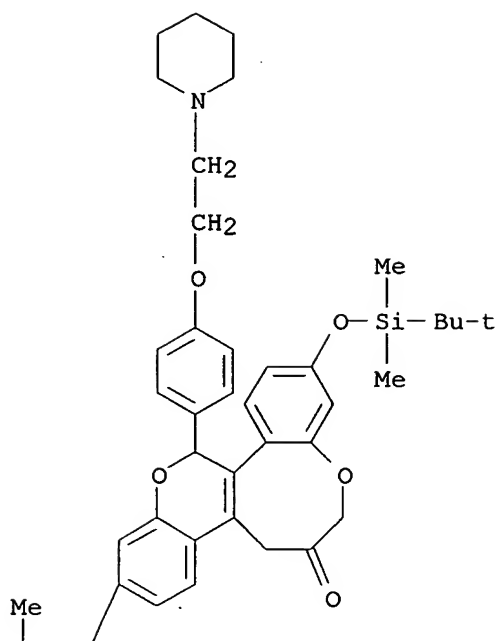


PAGE 2-A

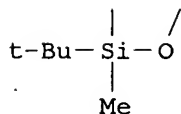


RN 554431-22-0 CAPLUS  
 CN [1]Benzopyrano[4,3-e][1]benzoxocin-6(7H)-one, 2,10-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,13-dihydro-13-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

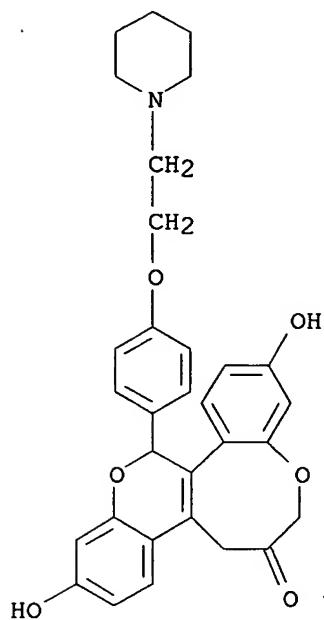


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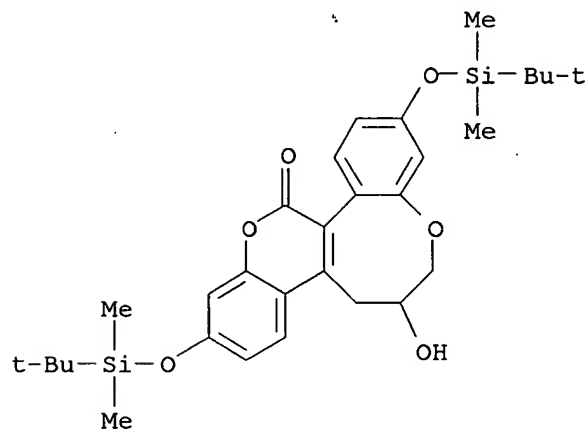
RN 554431-23-1 CAPLUS  
 CN [1]Benzopyrano[4,3-e][1]benzoxocin-6(7H)-one, .5,13-dihydro-2,10-dihydroxy-  
 13-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)





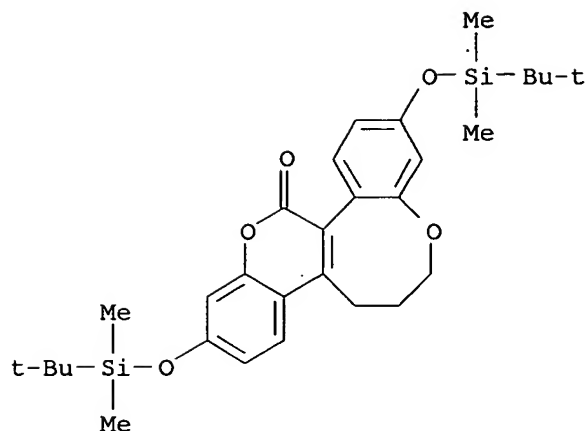
RN 554431-24-2 CAPLUS

CN [1]Benzopyrano[4,3-e][1]benzoxocin-13(5H)-one, 2,10-bis[[1,1-dimethylethyl]dimethylsilyl]oxy]-6,7-dihydro-6-hydroxy- (9CI) (CA INDEX NAME)



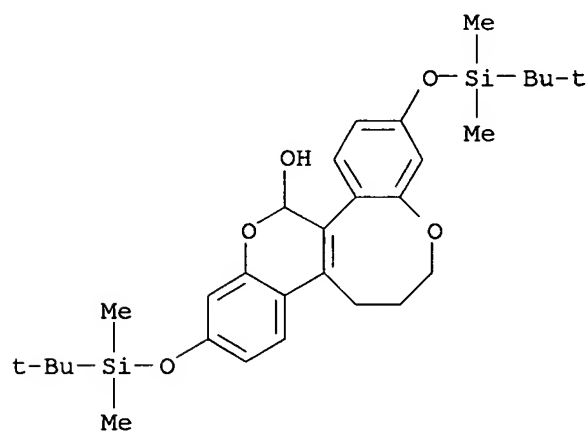
RN 554431-25-3 CAPLUS

CN [1]Benzopyrano[4,3-e][1]benzoxocin-13(5H)-one, 2,10-bis[[1,1-dimethylethyl]dimethylsilyl]oxy]-6,7-dihydro- (9CI) (CA INDEX NAME)



RN 554431-26-4 CAPLUS

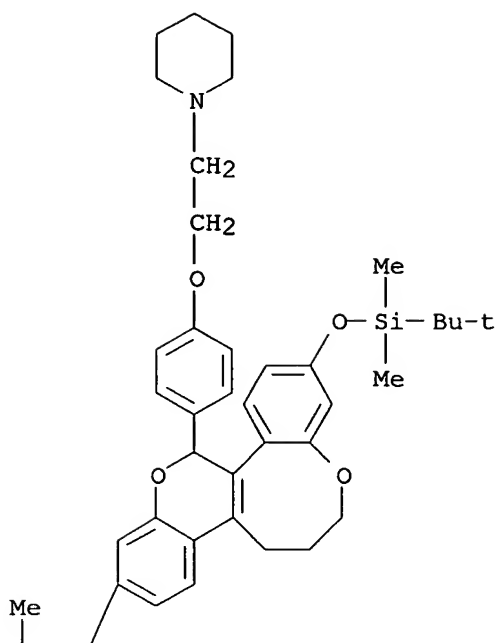
CN [1]Benzopyrano[4,3-e][1]benzoxocin-13-ol, 2,10-bis[[1,1-dimethylethyl]dimethylsilyl]oxy]-5,6,7,13-tetrahydro- (9CI) (CA INDEX NAME)



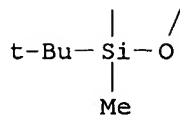
RN 554431-27-5 CAPLUS

CN Piperidine, 1-[2-[4-[2,10-bis[[1,1-dimethylethyl]dimethylsilyl]oxy]-5,6,7,13-tetrahydro[1]benzopyrano[4,3-e][1]benzoxocin-13-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

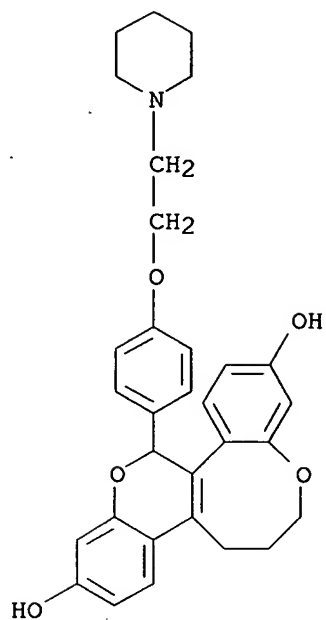


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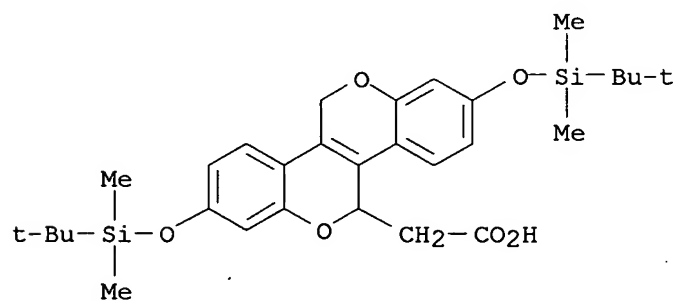
RN 554431-28-6 CAPLUS

CN [1]Benzopyrano[4,3-e][1]benzoxocin-2,10-diol, 5,6,7,13-tetrahydro-13-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



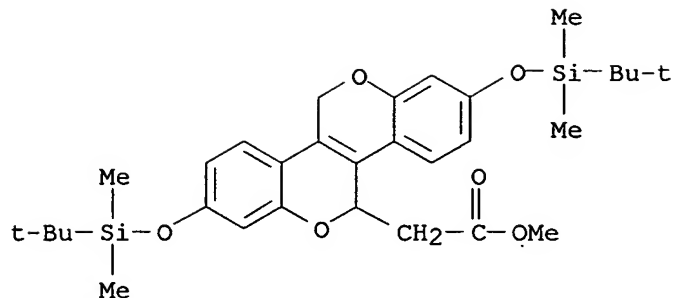
RN 554431-29-7 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5-acetic acid, 2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro- (9CI) (CA INDEX NAME)



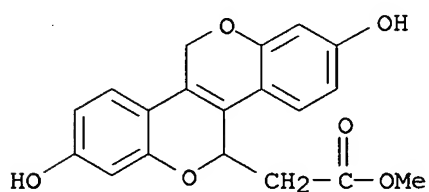
RN 554431-30-0 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5-acetic acid, 2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro-, methyl ester (9CI) (CA INDEX NAME)



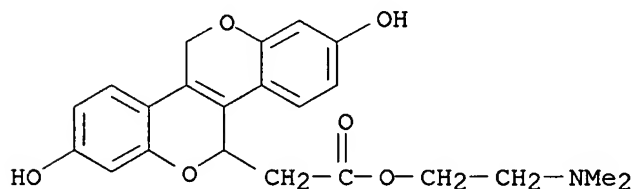
RN 554431-31-1 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5-acetic acid, 5,11-dihydro-2,8-dihydroxy-, methyl ester (9CI) (CA INDEX NAME)



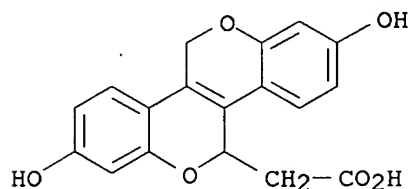
RN 554431-32-2 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5-acetic acid, 5,11-dihydro-2,8-dihydroxy-, 2-(dimethylamino)ethyl ester (9CI) (CA INDEX NAME)



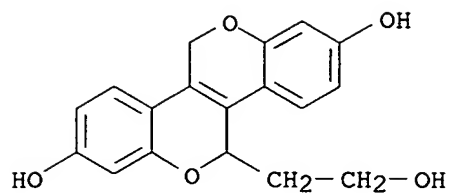
RN 554431-33-3 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5-acetic acid, 5,11-dihydro-2,8-dihydroxy- (9CI) (CA INDEX NAME)



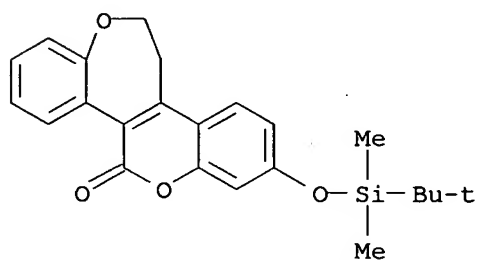
RN 554431-34-4 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)



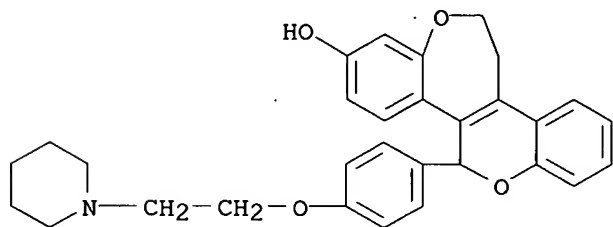
RN 554431-35-5 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 8-[[1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro- (9CI) (CA INDEX NAME)



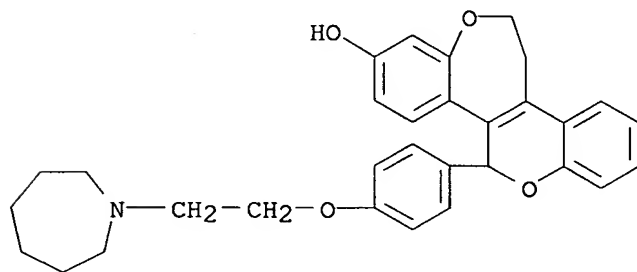
RN 554431-36-6 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 11,12-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



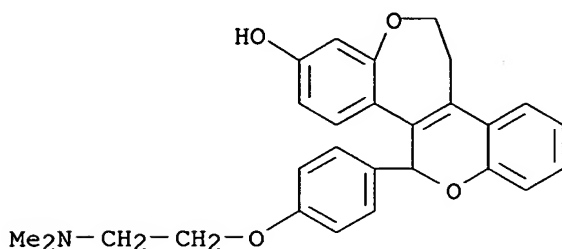
RN 554431-37-7 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro- (9CI) (CA INDEX NAME)



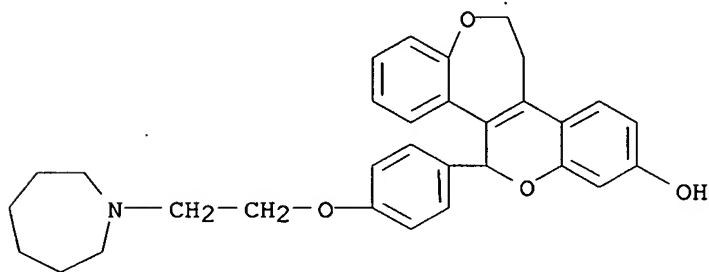
RN 554431-38-8 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 5-[4-[2-(dimethylamino)ethoxy]phenyl]-11,12-dihydro- (9CI) (CA INDEX NAME)



RN 554431-39-9 CAPLUS

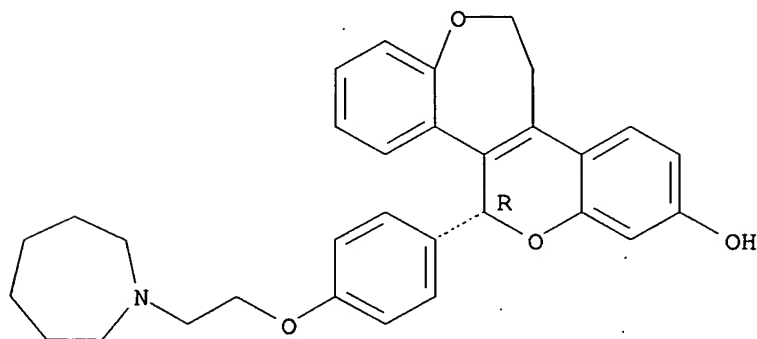
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-8-ol, 5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro- (9CI) (CA INDEX NAME)



RN 554431-40-2 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-8-ol, 5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro-, (5R)- (9CI) (CA INDEX NAME)

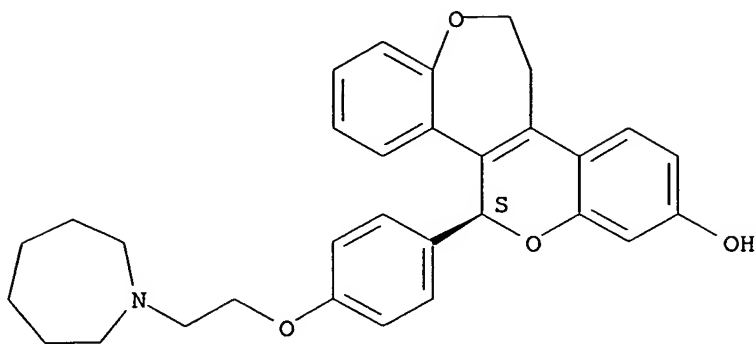
Absolute stereochemistry. Rotation (+).



RN 554431-41-3 CAPLUS

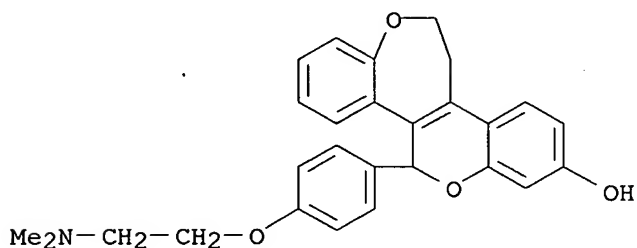
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-8-ol, 5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 554431-42-4 CAPLUS

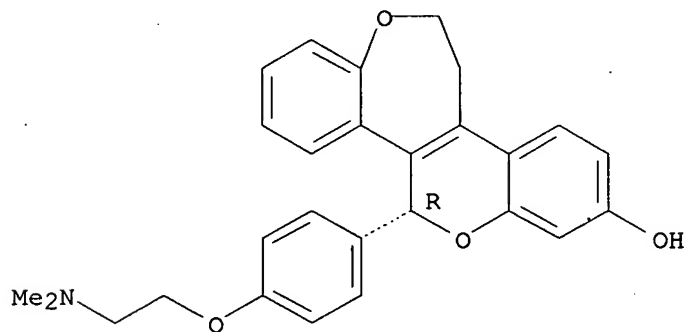
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-8-ol, 5-[4-[2-(dimethylamino)ethoxy]phenyl]-11,12-dihydro- (9CI) (CA INDEX NAME)



RN 554431-43-5 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-8-ol, 5-[4-[2-(dimethylamino)ethoxy]phenyl]-11,12-dihydro-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

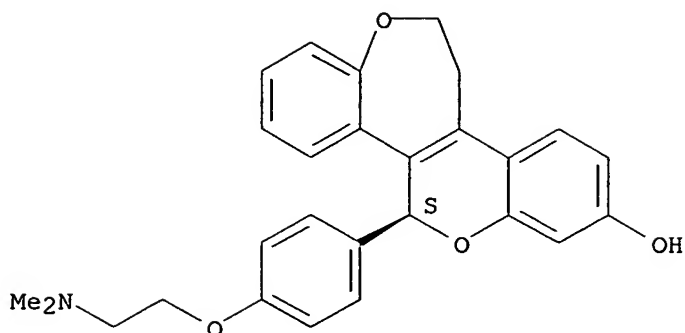


RN 554431-44-6 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-8-ol, 5-[4-[2-(dimethylamino)ethoxy]phenyl]-11,12-dihydro-, (5S)- (9CI) (CA INDEX NAME)

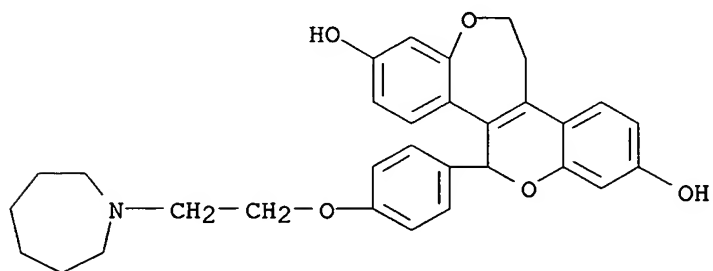
Absolute stereochemistry. Rotation (-).





RN 554431-45-7 CAPLUS

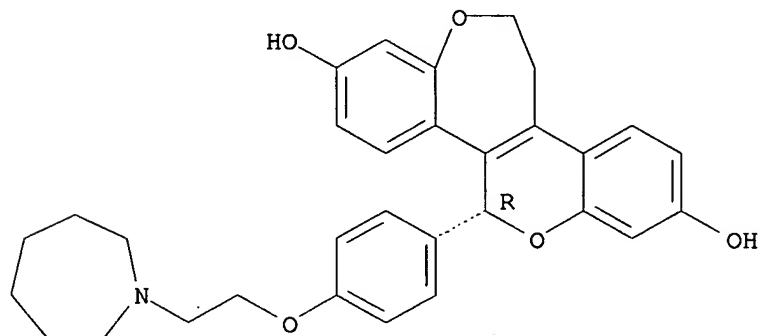
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro- (9CI) (CA INDEX NAME)



RN 554431-46-8 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro-, (5R)- (9CI) (CA INDEX NAME)

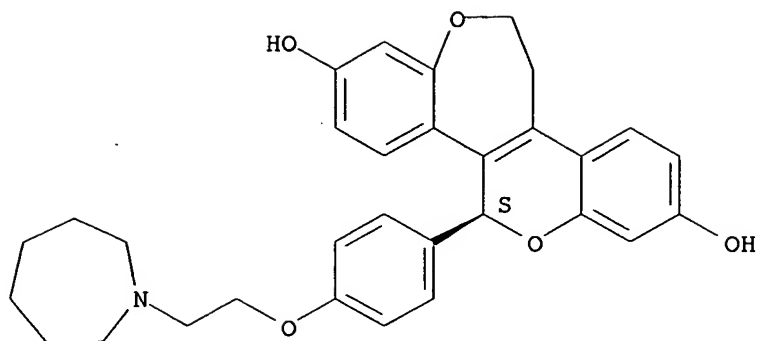
Absolute stereochemistry. Rotation (+).



RN 554431-47-9 CAPLUS

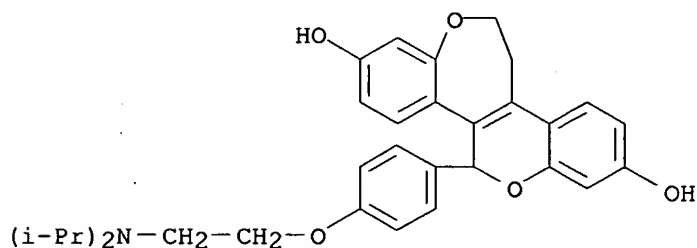
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-11,12-dihydro-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 554431-48-0 CAPLUS

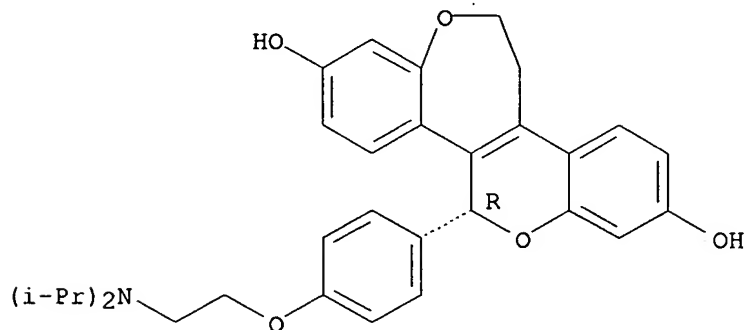
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 5-[4-[2-[bis(1-methylethyl)amino]ethoxy]phenyl]-11,12-dihydro- (9CI) (CA INDEX NAME)



RN 554431-49-1 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 5-[4-[2-[bis(1-methylethyl)amino]ethoxy]phenyl]-11,12-dihydro-, (5R)- (9CI) (CA INDEX NAME)

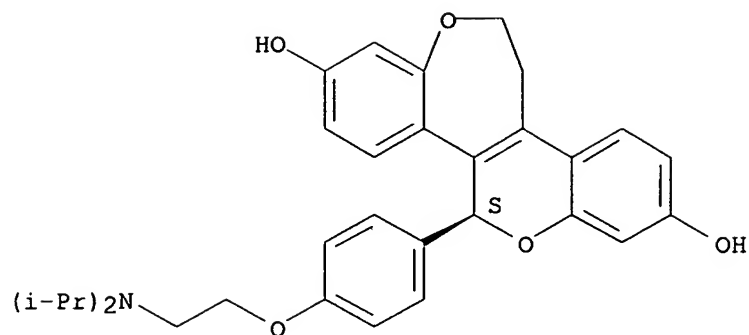
Absolute stereochemistry. Rotation (+).



RN 554431-50-4 CAPLUS

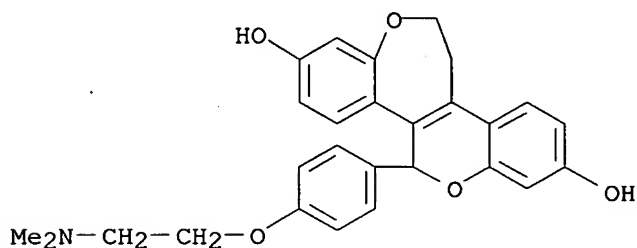
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 5-[4-[2-[bis(1-methylethyl)amino]ethoxy]phenyl]-11,12-dihydro-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 554431-51-5 CAPLUS

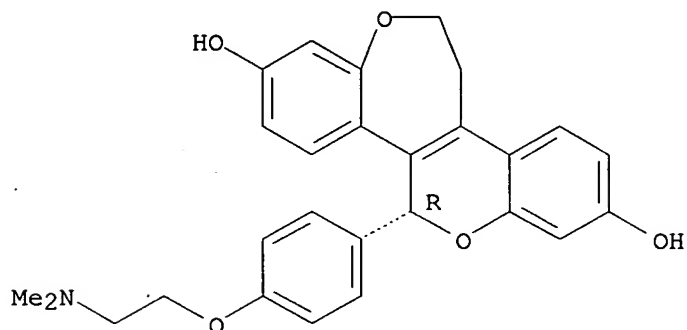
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 5-[4-[2-(dimethylamino)ethoxy]phenyl]-11,12-dihydro- (9CI) (CA INDEX NAME)



RN 554431-52-6 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 5-[4-[2-(dimethylamino)ethoxy]phenyl]-11,12-dihydro-, (5R)- (9CI) (CA INDEX NAME)

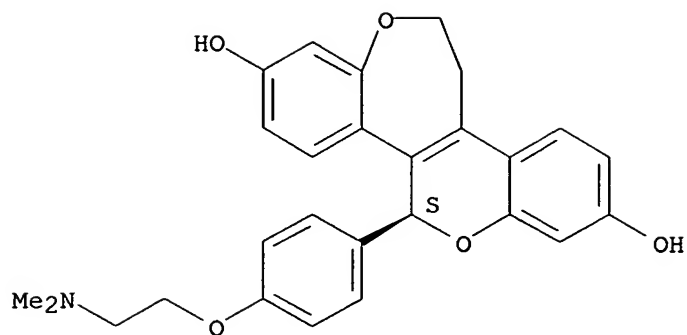
Absolute stereochemistry. Rotation (+).



RN 554431-53-7 CAPLUS

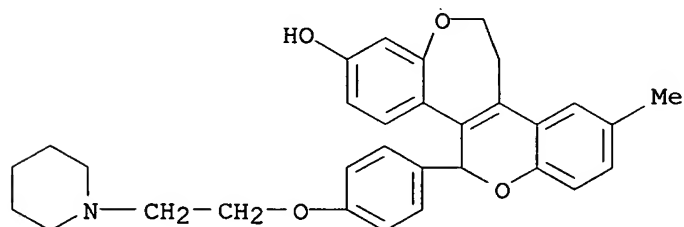
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 5-[4-[2-(dimethylamino)ethoxy]phenyl]-11,12-dihydro-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



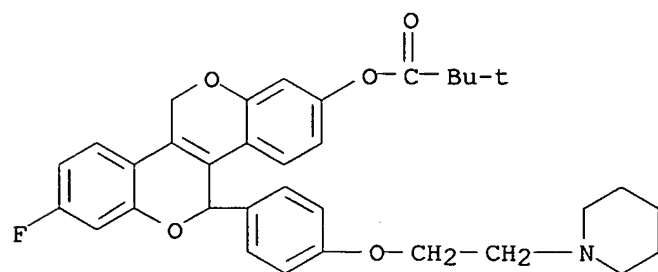
RN 554431-54-8 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 11,12-dihydro-9-methyl-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



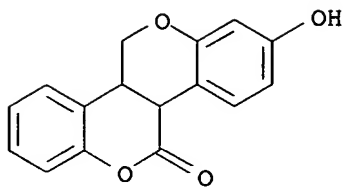
RN 554431-55-9 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 8-fluoro-5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2-yl ester (9CI) (CA INDEX NAME)



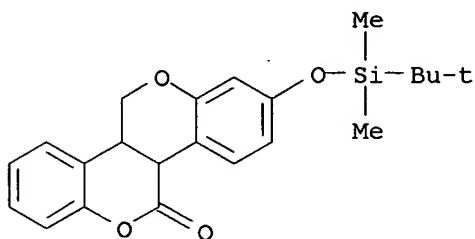
RN 554431-56-0 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5(4bH)-one, 10b,11-dihydro-2-hydroxy- (9CI) (CA INDEX NAME)



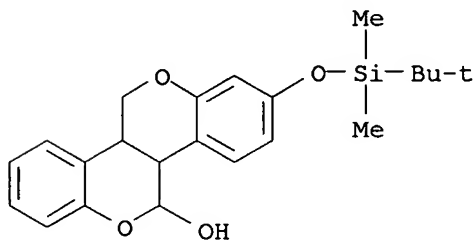
RN 554431-57-1 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5(4bH)-one, 2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-10b,11-dihydro- (9CI) (CA INDEX NAME)



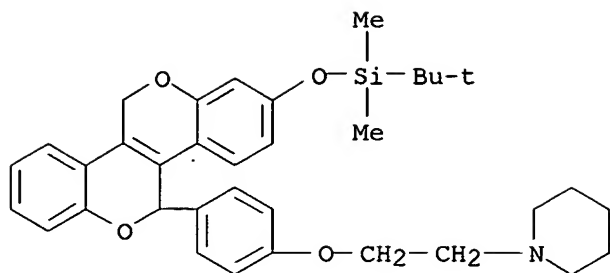
RN 554431-58-2 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5-ol, 2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4b,5,10b,11-tetrahydro- (9CI) (CA INDEX NAME)



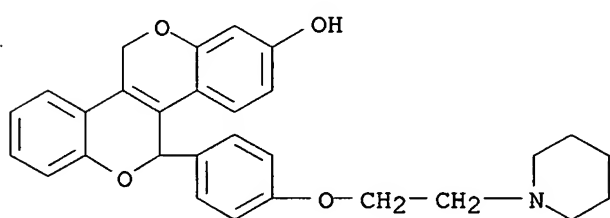
RN 554431-59-3 CAPLUS

CN Piperidine, 1-[2-[4-[2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



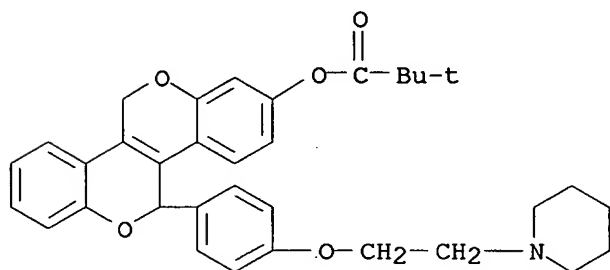
RN 554431-60-6 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2-ol, 5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



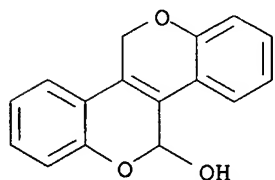
RN 554431-61-7 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2-yl ester (9CI) (CA INDEX NAME)



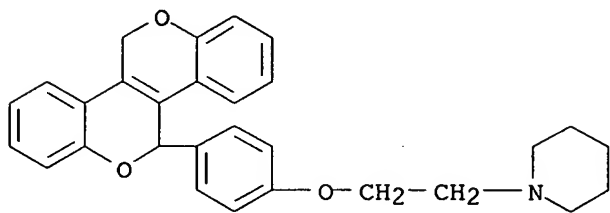
RN 554431-62-8 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5-ol, 5,11-dihydro- (9CI) (CA INDEX NAME)



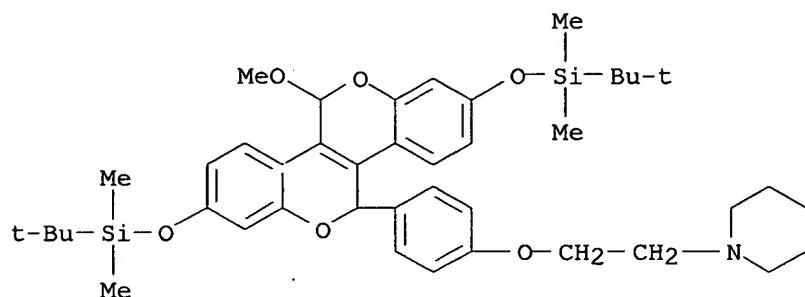
RN 554431-63-9 CAPLUS

CN Piperidine, 1-[2-[4-(5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl)phenoxy]ethyl]- (9CI) (CA INDEX NAME)



RN 554431-64-0 CAPLUS

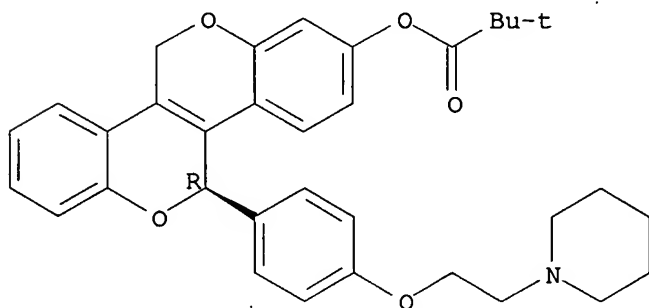
CN Piperidine, 1-[2-[4-[2,8-bis[[ (1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro-11-methoxy[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



RN 554431-65-1 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, (5R)-5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

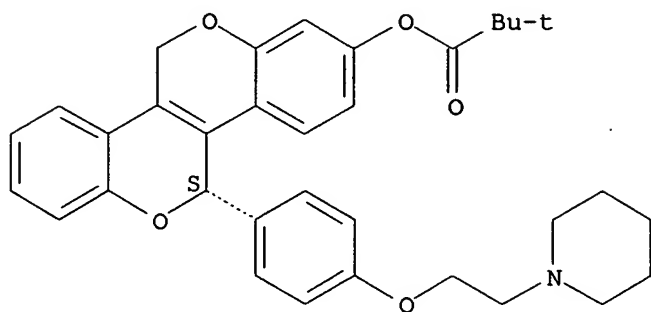


RN 554431-66-2 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, (5S)-5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2-yl ester (9CI) (CA INDEX NAME)

10/307,735

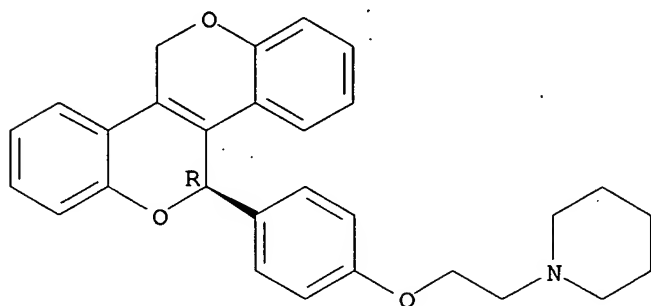
Absolute stereochemistry. Rotation (+).



RN 554431-67-3 CAPLUS

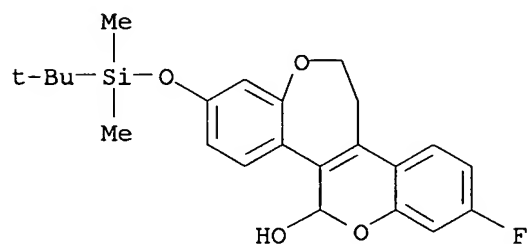
CN Piperidine, 1-[2-[4-[(5R)-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 554431-68-4 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-ol, 2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-fluoro-11,12-dihydro- (9CI) (CA INDEX NAME)

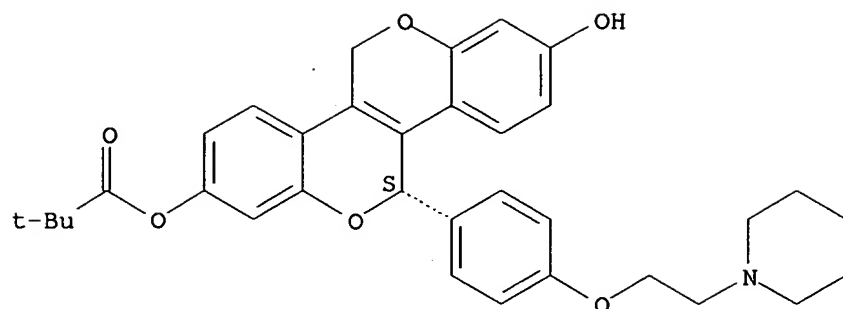


RN 554431-69-5 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, (11S)-5,11-dihydro-8-hydroxy-11-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

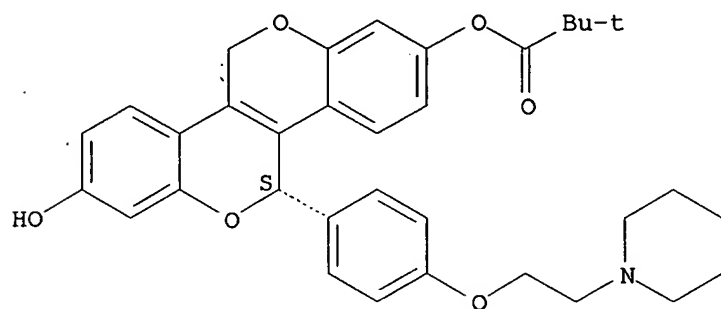




RN 554431-70-8 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, (5S)-5,11-dihydro-8-hydroxy-5-[4-[3-(1-piperidinyl)propoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2-yl ester (9CI) (CA INDEX NAME)

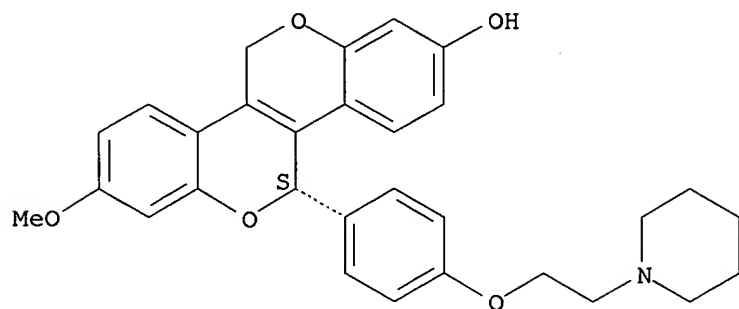
Absolute stereochemistry. Rotation (+).



RN 554431-71-9 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2-ol, 5,11-dihydro-8-methoxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (5S)- (9CI) (CA INDEX NAME)

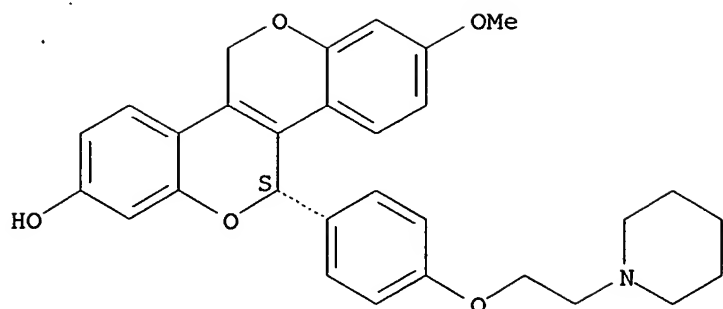
Absolute stereochemistry.



RN 554431-72-0 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2-ol, 5,11-dihydro-8-methoxy-11-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (11S)- (9CI) (CA INDEX NAME)

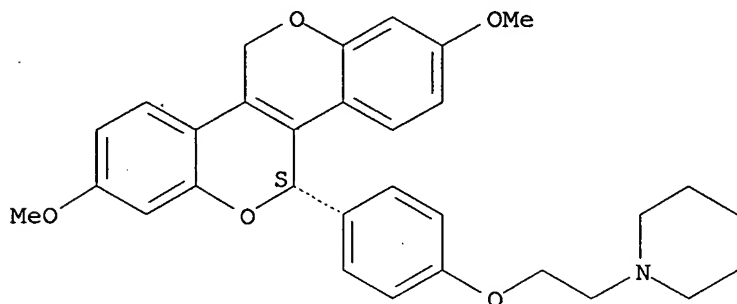
Absolute stereochemistry. Rotation (-).



RN 554431-73-1 CAPLUS

CN Piperidine, 1-[2-[4-[(5S)-5,11-dihydro-2,8-dimethoxy[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

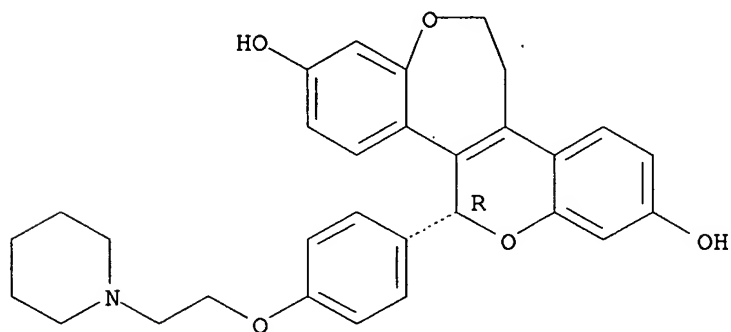
Absolute stereochemistry. Rotation (+).



RN 554431-74-2 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 11,12-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (5R)- (9CI) (CA INDEX NAME)

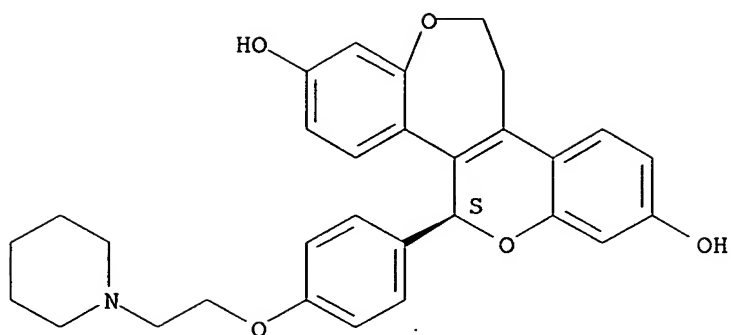
Absolute stereochemistry. Rotation (+).



RN 554431-75-3 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2,8-diol, 11,12-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (5S)- (9CI) (CA INDEX NAME)

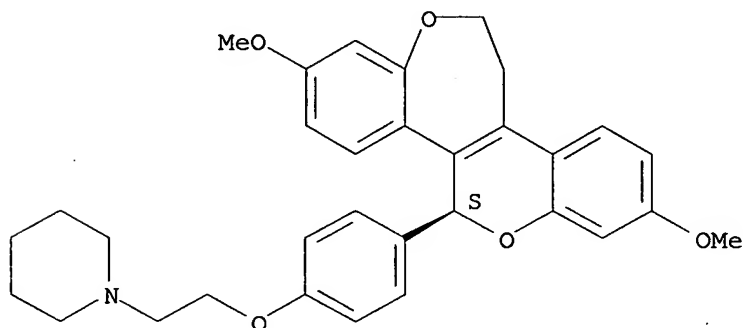
Absolute stereochemistry. Rotation (-).



RN 554431-76-4 CAPLUS

CN Piperidine, 1-[2-[4-[(5S)-11,12-dihydro-2,8-dimethoxy-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

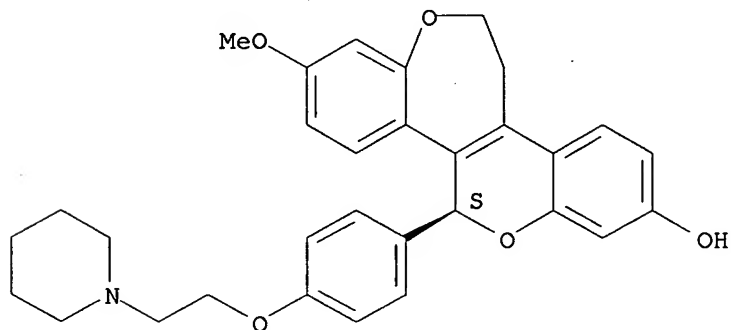
Absolute stereochemistry. Rotation (-).



RN 554431-77-5 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-8-ol, 11,12-dihydro-2-methoxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (5S)- (9CI) (CA INDEX NAME)

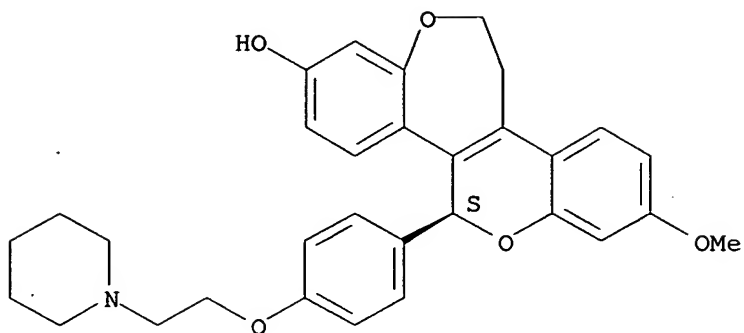
Absolute stereochemistry. Rotation (-).



RN 554431-78-6 CAPLUS

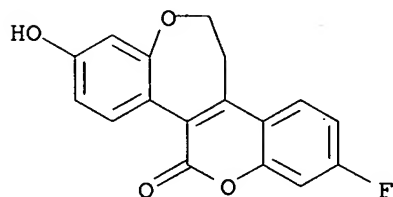
CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-2-ol, 11,12-dihydro-8-methoxy-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



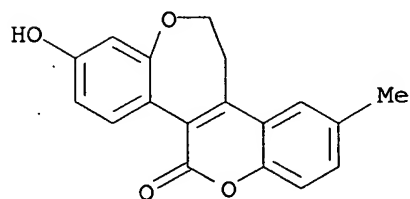
RN 554431-79-7 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 8-fluoro-11,12-dihydro-2-hydroxy- (9CI) (CA INDEX NAME)



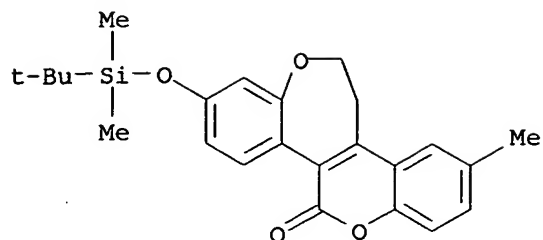
RN 554431-80-0 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 11,12-dihydro-2-hydroxy-9-methyl- (9CI) (CA INDEX NAME)



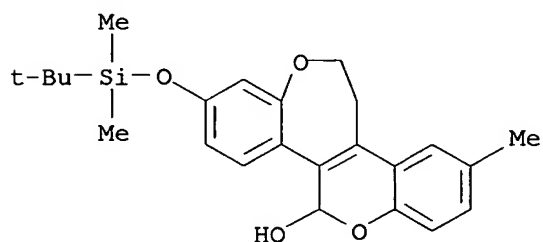
RN 554431-81-1 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro-9-methyl- (9CI) (CA INDEX NAME)



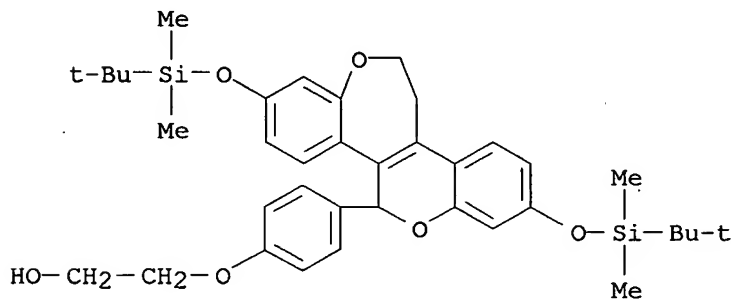
RN 554431-82-2 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-ol, 2-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro-9-methyl- (9CI) (CA INDEX NAME)



RN 554431-83-3 CAPLUS

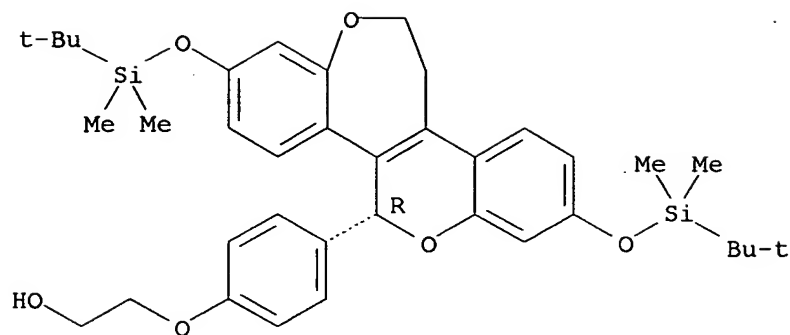
CN Ethanol, 2-[4-[2,8-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]- (9CI) (CA INDEX NAME)



RN 554431-84-4 CAPLUS

CN Ethanol, 2-[4-[(5R)-2,8-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]- (9CI) (CA INDEX NAME)

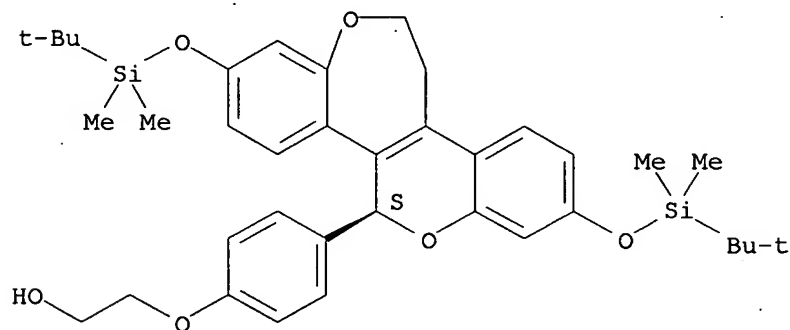
Absolute stereochemistry. Rotation (+).



RN 554431-85-5 CAPLUS

CN Ethanol, 2-[4-[(5S)-2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]- (9CI) (CA INDEX NAME)

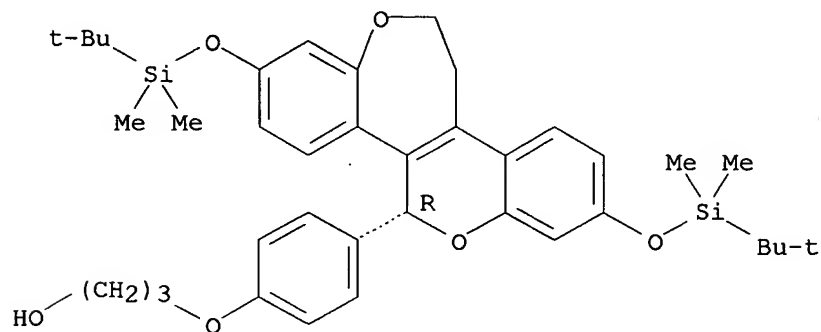
Absolute stereochemistry. Rotation (-).



RN 554431-86-6 CAPLUS

CN 1-Propanol, 3-[4-[(5R)-2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

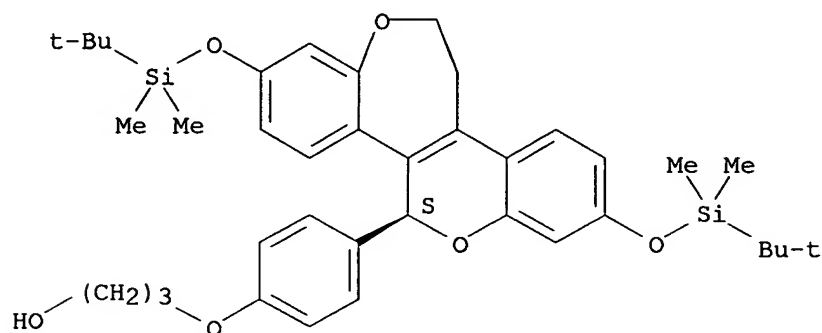


RN 554431-87-7 CAPLUS

10/307,735

CN 1-Propanol, 3-[4-[(5S)-2,8-bis[[ (1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]- (9CI)  
(CA INDEX NAME)

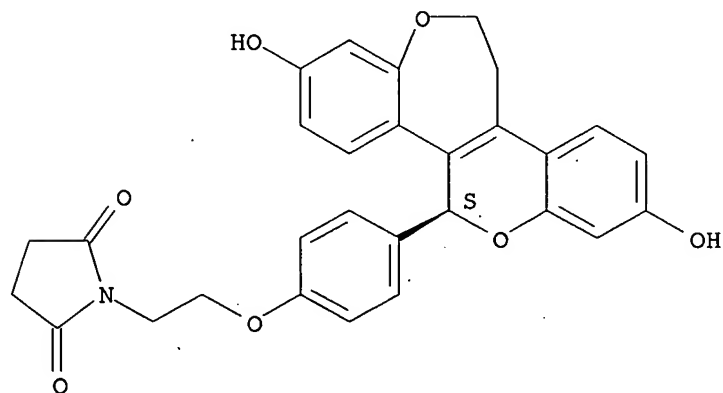
Absolute stereochemistry. Rotation (-).



RN 554431-88-8 CAPLUS

CN 2,5-Pyrrolidinedione, 1-[2-[4-[(5S)-11,12-dihydro-2,8-dihydroxy-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

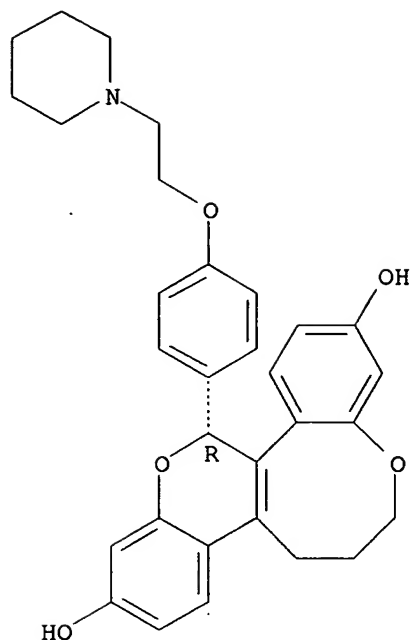
Absolute stereochemistry. Rotation (+).



RN 554431-92-4 CAPLUS

CN [1]Benzopyrano[4,3-e][1]benzoxocin-2,10-diol, 5,6,7,13-tetrahydro-13-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (13R)- (9CI) (CA INDEX NAME)

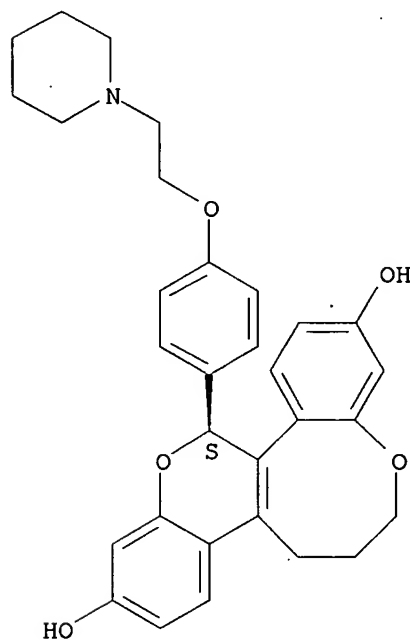
Absolute stereochemistry. Rotation (-).



RN 554431-93-5 CAPLUS

CN [1]Benzopyrano[4,3-e][1]benzoxocin-2,10-diol, 5,6,7,13-tetrahydro-13-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (13S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

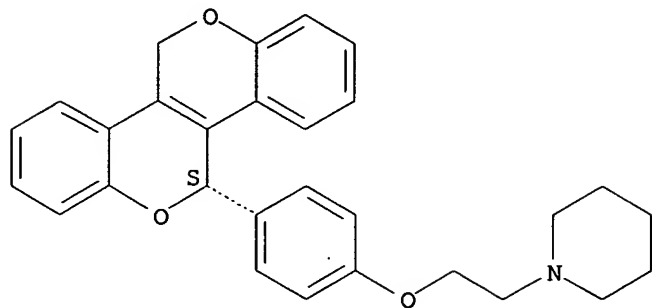


RN 554433-05-5 CAPLUS

CN Piperidine, 1-[2-[4-[(5S)-5,11-dihydro[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

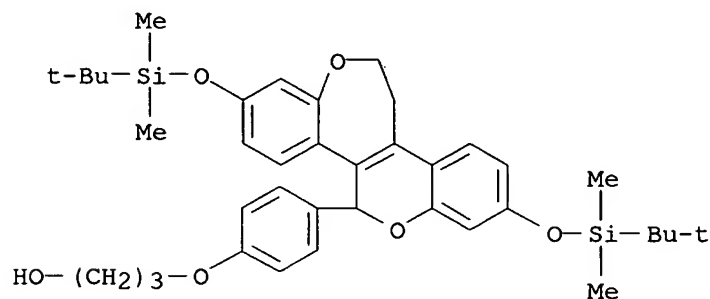


Absolute stereochemistry. Rotation (+).



RN 554433-06-6 CAPLUS

CN 1-Propanol, 3-[4-[2,8-bis[[[1,1-dimethylethyl]dimethylsilyl]oxy]-11,12-dihydro-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]- (9CI) (CA INDEX NAME)



IT 553681-47-3 554430-69-2 554430-70-5

554430-71-6 554430-72-7 554430-73-8

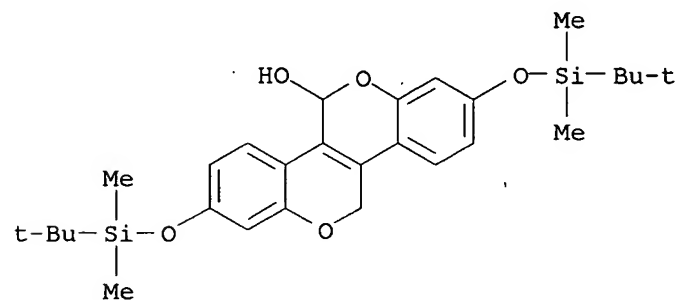
554430-74-9 554430-75-0 554430-77-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of tetracyclic heterocycles as selective estrogen receptor modulators (SERMs))

RN 553681-47-3 CAPLUS

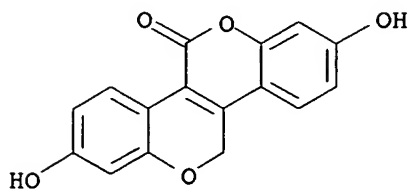
CN [1]Benzopyrano[4,3-c][1]benzopyran-5-ol, 2,8-bis[[[1,1-dimethylethyl]dimethylsilyl]oxy]-5,11-dihydro- (9CI) (CA INDEX NAME)



RN 554430-69-2 CAPLUS

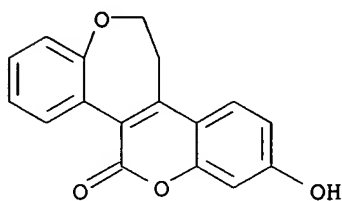
10/307,735

CN [1]Benzopyrano[4,3-c][1]benzopyran-5(11H)-one, 2,8-dihydroxy- (9CI) (CA INDEX NAME)



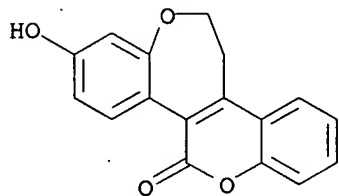
RN 554430-70-5 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 11,12-dihydro-8-hydroxy- (9CI) (CA INDEX NAME)



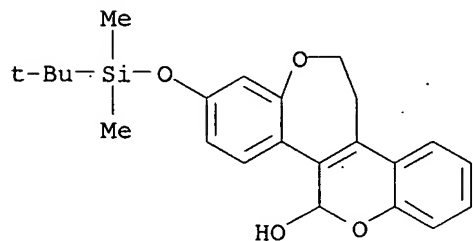
RN 554430-71-6 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 11,12-dihydro-2-hydroxy- (9CI) (CA INDEX NAME)



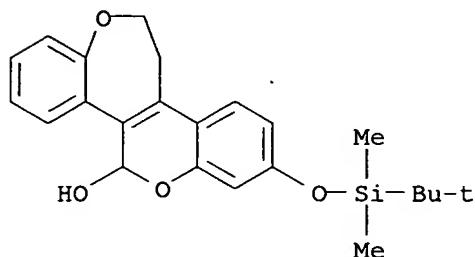
RN 554430-72-7 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-ol, 2-[[ (1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro- (9CI) (CA INDEX NAME)



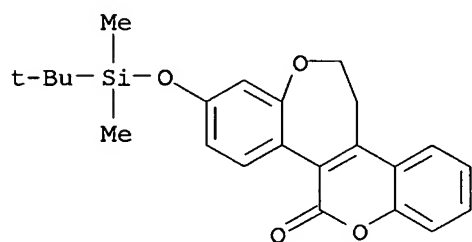
RN 554430-73-8 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-ol, 8-[[ (1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro- (9CI) (CA INDEX NAME)



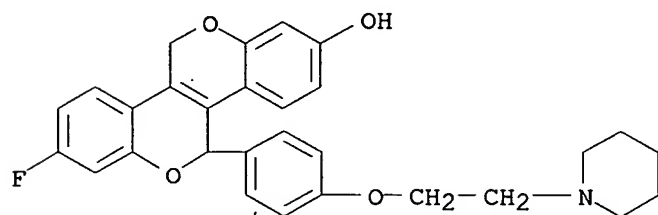
RN 554430-74-9 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 2-[[ (1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro- (9CI) (CA INDEX NAME)



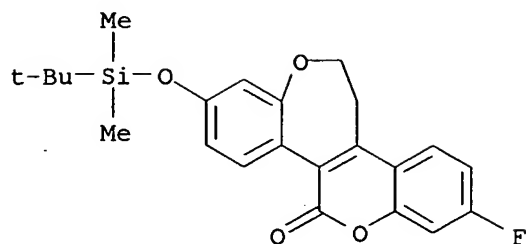
RN 554430-75-0 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2-ol, 8-fluoro-5,11-dihydro-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



RN 554430-77-2 CAPLUS

CN 5H-[1]Benzopyrano[4,3-d][1]benzoxepin-5-one, 2-[[ (1,1-dimethylethyl)dimethylsilyl]oxy]-8-fluoro-11,12-dihydro- (9CI) (CA INDEX NAME)

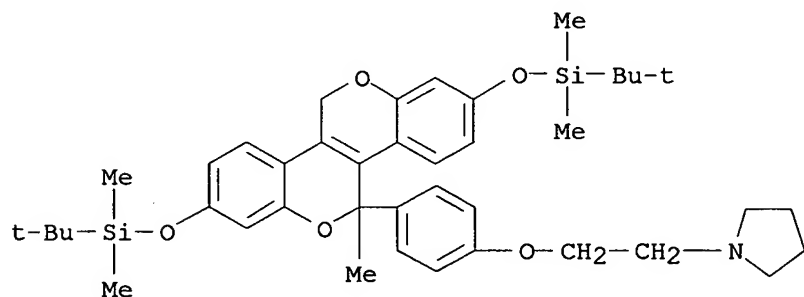


IT 554430-22-7P 554430-23-8P 554430-25-0P  
 554430-26-1P 554430-28-3P 554430-29-4P  
 554430-31-8P 554430-32-9P 554430-34-1P  
 554430-35-2P 554430-50-1P 554430-51-2P  
 554430-52-3P 554431-90-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of tetracyclic heterocycles as selective estrogen receptor  
 modulators (SERMs))

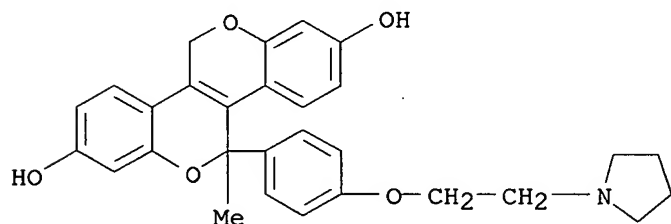
RN 554430-22-7 CAPLUS

CN Silane, [[5,11-dihydro-5-methyl-5-[4-[2-(1-pyrrolidinyl)ethoxy]phenyl][1]b  
 enzopyrano[4,3-c][1]benzopyran-2,8-diyl]bis(oxy)]bis[(1,1-  
 dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



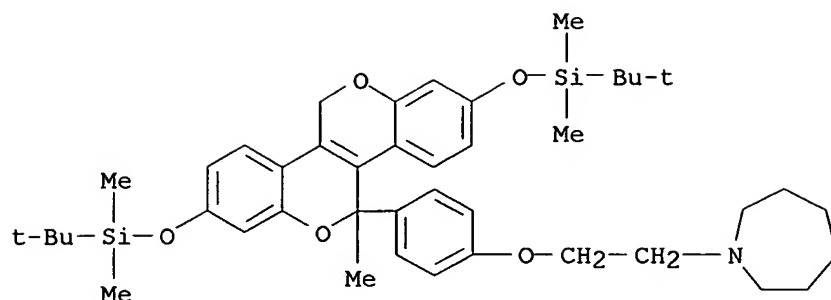
RN 554430-23-8 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-methyl-5-[4-[2-  
 (1-pyrrolidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



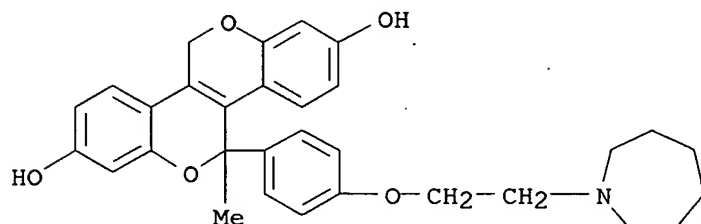
RN 554430-25-0 CAPLUS

CN Silane, [[5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-5,11-dihydro-5-  
 methyl[1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl]bis(oxy)]bis[(1,1-  
 dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



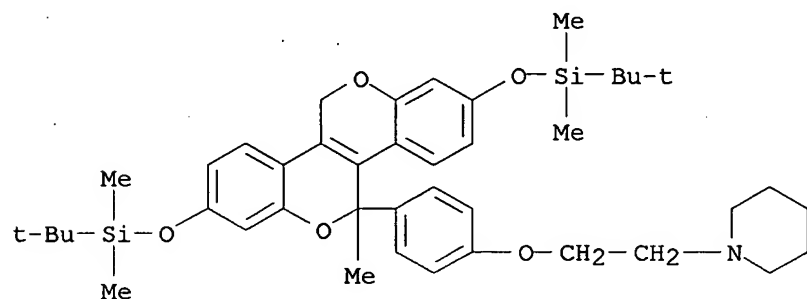
RN 554430-26-1 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5-[4-[2-(hexahydro-1H-azepin-1-yl)ethoxy]phenyl]-5,11-dihydro-5-methyl- (9CI) (CA INDEX NAME)



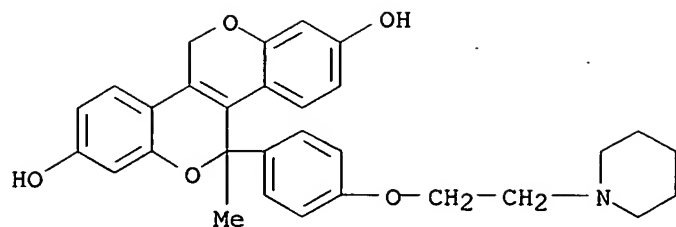
RN 554430-28-3 CAPLUS

CN Silane, [[5,11-dihydro-5-methyl-5-[4-[2-(1-piperidinyl)ethoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



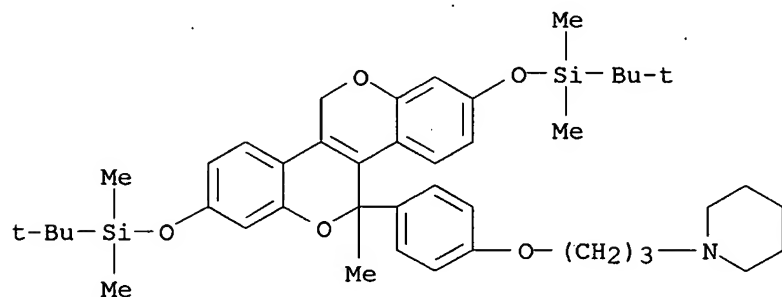
RN 554430-29-4 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-methyl-5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



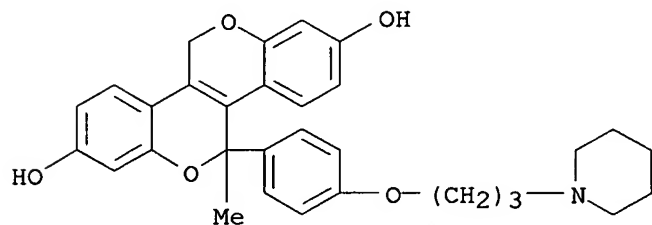
RN 554430-31-8 CAPLUS

CN Silane, [[5,11-dihydro-5-methyl-5-[4-[3-(1-piperidinyl)propoxy]phenyl][1]benzopyrano[4,3-c][1]benzopyran-2,8-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



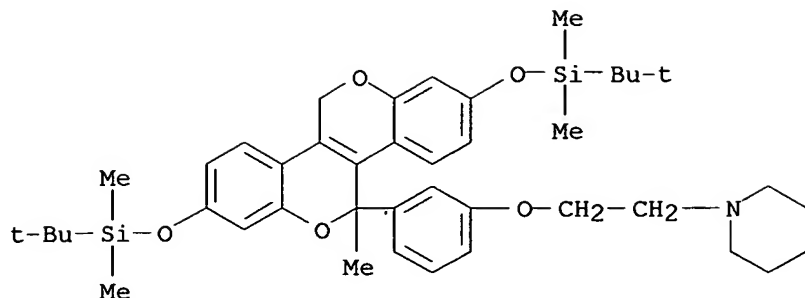
RN 554430-32-9 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-methyl-5-[4-[3-(1-piperidinyl)propoxy]phenyl]- (9CI) (CA INDEX NAME)



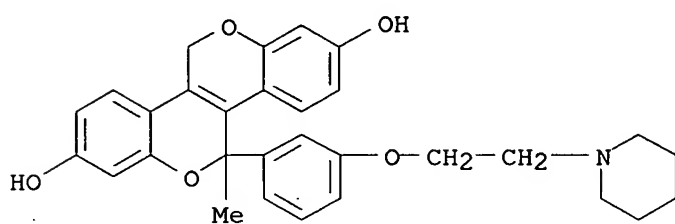
RN 554430-34-1 CAPLUS

CN Piperidine, 1-[2-[3-[2,8-bis[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro-5-methyl[1]benzopyrano[4,3-c][1]benzopyran-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



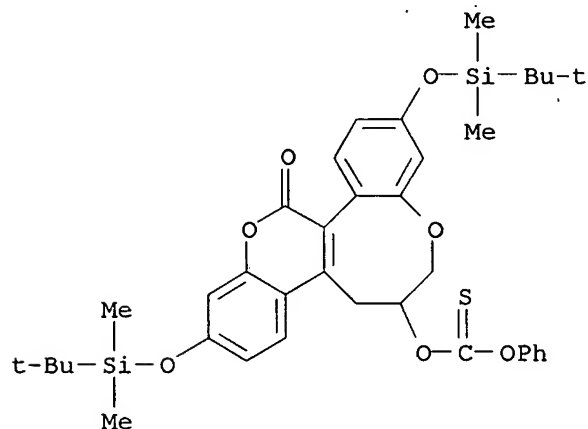
RN 554430-35-2 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-2,8-diol, 5,11-dihydro-5-methyl-5-[3-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



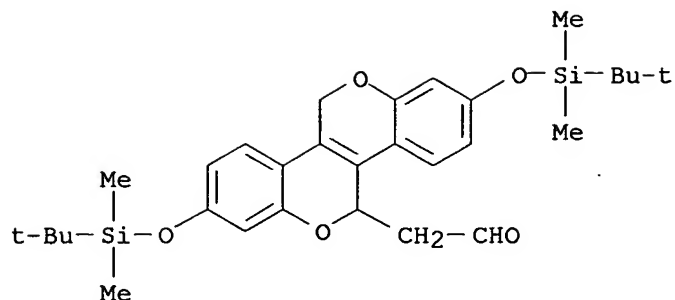
RN 554430-50-1 CAPLUS

CN Carbonothioic acid, O-[2,10-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,6,7,13-tetrahydro-13-oxo[1]benzopyrano[4,3-e][1]benzoxocin-6-yl] O-phenyl ester (9CI) (CA INDEX NAME)



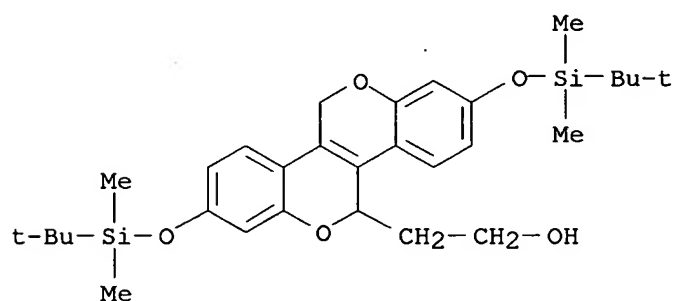
RN 554430-51-2 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5-acetaldehyde, 2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,11-dihydro- (9CI) (CA INDEX NAME)



RN 554430-52-3 CAPLUS

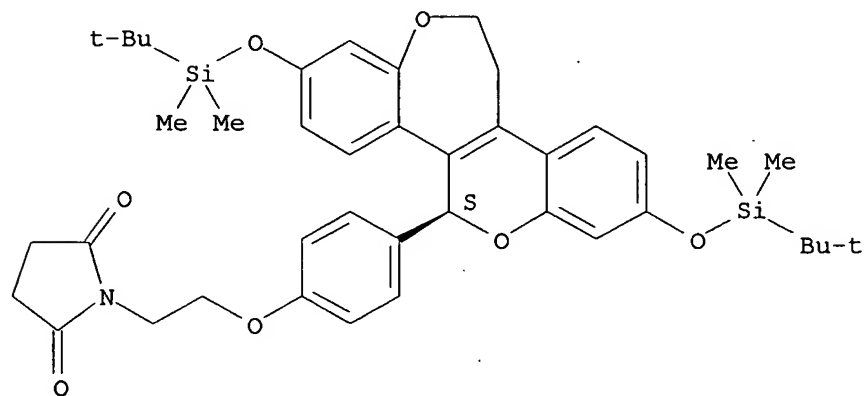
CN [1]Benzopyrano[4,3-c][1]benzopyran-5-ethanol, 2,8-bis[((1,1-dimethylethyl)dimethylsilyl)oxy]-5,11-dihydro- (9CI) (CA INDEX NAME)



RN 554431-90-2 CAPLUS

CN 2,5-Pyrrolidinedione, 1-[2-[4-[(5S)-2,8-bis[((1,1-dimethylethyl)dimethylsilyl)oxy]-11,12-dihydro-5H-[1]benzopyrano[4,3-d][1]benzoxepin-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT:

3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



✓ 122 ANSWER 11 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:498000 CAPLUS

DOCUMENT NUMBER: 139:176251

TITLE: BHB: A simple knowledge-based scoring function to improve the efficiency of database screening

AUTHOR(S): Feher, Miklos; Deretey, Eugen; Roy, Samir

CORPORATE SOURCE: SignalGene Inc., Guelph, ON, N1G 4P7, Can.

SOURCE: Journal of Chemical Information and Computer Sciences (2003), 43(4), 1316-1327  
CODEN: JCISD8; ISSN: 0095-2338

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new knowledge-based scoring function was developed in this work to facilitate the rapid ranking of ligands in databases. The acronym of the method is BHB based on the descriptors it utilizes: buriedness, hydrogen bonding, and binding energy. Receptor buriedness is a measure of how well mols. occupy the binding pocket in comparison to known high-affinity ligands or, alternatively, whether they have contact with identified residues in the pocket. The possibility of hydrogen bond formation is checked for selected residues that are recognized as being important in the binding of known ligands. The approx. binding energy is calculated from the thermodyn. cycle using the optimized bound and free solvent conformations of the ligand-receptor system. The information necessary for the scoring function can ideally be gleaned from the 3D structure of the receptor-ligand complex. Alternatively, the descriptors can be derived from the 3D structure of the unbound receptor, provided this receptor has a known ligand that binds to the given site with nanomolar activity. We show that the new scoring functions provide up to 12 times improvement in enrichment compared to the popular com. docking program GOLD.

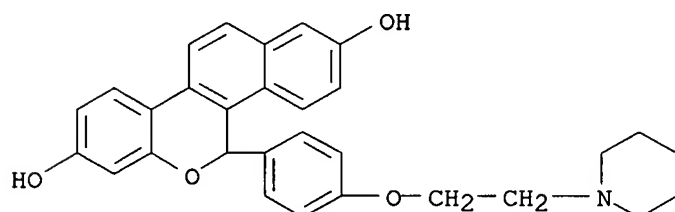
IT 188824-17-1, LY-357489

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(BHB knowledge-based scoring function to improve the efficiency of database screening)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol, 5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

50

THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

X22 ANSWER 12 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:192085 CAPLUS

DOCUMENT NUMBER: 139:52971

TITLE: Regioselective synthesis of 1H,3H,6H[2]benzopyrano[4,3-d]pyrimidine-2,4-diones and 12H-benzopyrano[3,2-c][1]benzopyran-5-ones by radical cyclization

AUTHOR(S): Majumdar, K. C.; Basu, P. K.; Mukhopadhyay, P. P.; Sarkar, S.; Ghosh, S. K.; Biswas, P.

CORPORATE SOURCE: Department of Chemistry, University of Kalyani, Kalyani, 741 235, India

SOURCE: Tetrahedron (2003), 59(12), 2151-2157

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:52971

AB 5-Hydroxy uracils or 4-hydroxy[1]benzopyran-2-ones were refluxed with 2-bromobenzyl bromides in acetone in the presence of anhydrous potassium carbonate to afford a number of 5-(2'-bromobenzoyloxy) pyrimidine-2,4-dione (80-92%) or 4-(2'-bromobenzoyloxy) benzopyran-7-ones (70-82%) resp. These were then refluxed with tri-n-butyltin chloride and sodium cyanoborohydride in the presence of a catalytic amount of azobisisobutyronitrile (AIBN) for 3-4 h to give 1H,3H,6H [2]benzopyrano[4,3-d]pyrimidine-2,4-diones (75-85%) or 12H-benzopyrano[3,2-c][1]benzopyran-5-ones (70-85%) resp.

IT 96600-94-1P 545402-65-1P 545402-66-2P

545402-67-3P 545402-68-4P 545402-69-5P

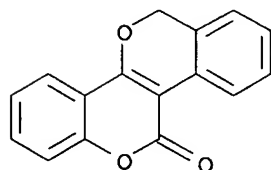
545402-70-8P 545402-71-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(regioselective preparation of 1H,3H,6H[2]benzopyrano[4,3-d]pyrimidine-2,4-diones and 12H-benzopyrano[3,2-c][1]benzopyran-5-ones)

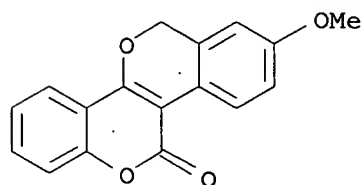
RN 96600-94-1 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-11-one (9CI) (CA INDEX NAME)



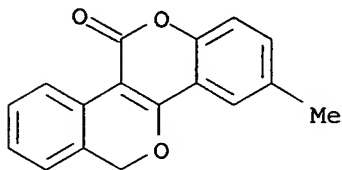
RN 545402-65-1 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-11-one, 8-methoxy- (9CI) (CA INDEX NAME)



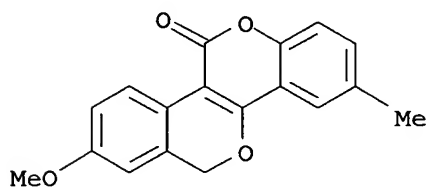
RN 545402-66-2 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-11-one, 3-methyl- (9CI) (CA INDEX NAME)



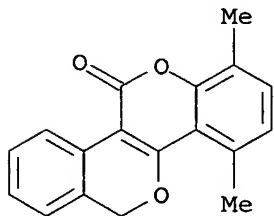
RN 545402-67-3 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-11-one, 8-methoxy-3-methyl- (9CI) (CA INDEX NAME)



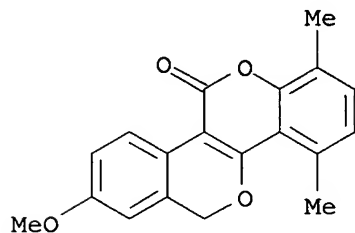
RN 545402-68-4 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-11-one, 1,4-dimethyl- (9CI) (CA INDEX NAME)



RN 545402-69-5 CAPLUS

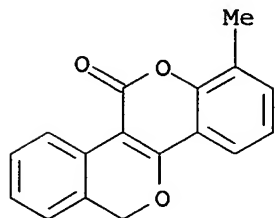
CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-11-one, 8-methoxy-1,4-dimethyl- (9CI) (CA INDEX NAME)



RN 545402-70-8 CAPLUS

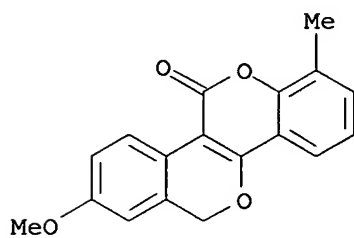
CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-11-one, 1-methyl- (9CI) (CA INDEX NAME)

INDEX NAME)



RN 545402-71-9 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-11-one, 8-methoxy-1-methyl-  
(9CI) (CA INDEX NAME)



REFERENCE COUNT:

56

THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

122 ANSWER 13 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:940242 CAPLUS

DOCUMENT NUMBER: 137:380017

TITLE: Estrogen receptor  $\beta$ -based hypertension treatment and assay

INVENTOR(S): Gustafsson, Jan-Ake; Bian, Zhao

PATENT ASSIGNEE(S): Karo Bio AB, Swed.

SOURCE: Brit. UK Pat. Appl., 28 pp.

CODEN: BAXXDU

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2374412	A1	20021016	GB 2001-9091	20010411
PRIORITY APPLN. INFO.:			GB 2001-9091	20010411

AB Methods are disclosed for assaying compds. for blood pressure-modulating activity. The methods include determining the ability of the compound to affect

estrogen receptor  $\beta$  (ER $\beta$ ) activity. The invention also discloses the use of ER $\beta$ -modulating compds. for modulating blood pressure, in particular for treating hypertension.

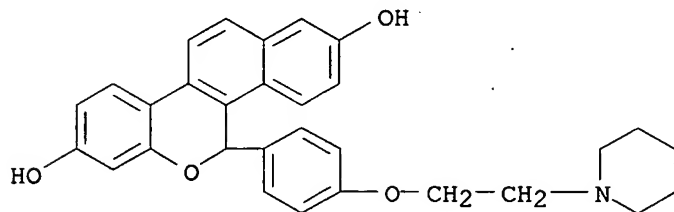
IT 188824-17-1, LY-357489

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(estrogen receptor  $\beta$ -based hypertension treatment and assay)

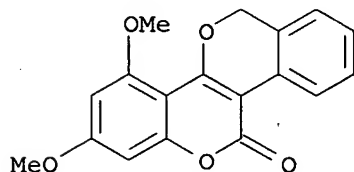
RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol, 5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



~~12~~ ANSWER 14 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:808688 CAPLUS  
 DOCUMENT NUMBER: 138:237974  
 TITLE: Three-step one-pot organobismuth-mediated synthesis of benzo[b]pyran compounds  
 AUTHOR(S): Bolshakov, Alexey V.; Ganina, Olga G.; Shavirin, Andrew S.; Kurskii, Yury A.; Finet, Jean-Pierre; Fedorov, Alexey Yu.  
 CORPORATE SOURCE: Department of Organic Chemistry, Nizhny Novgorod State University, Nizhny Novgorod, 603950, Russia  
 SOURCE: Tetrahedron Letters (2002), 43(46), 8245-8248  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 138:237974  
 AB Tris[o-chloromethylphenyl]bismuth diacetate reacted with phenols and enolizable substrates in the presence of a base to afford good yields of oxaphenanthrene derivs. This bismuth-mediated oxidation/o-arylation/cyclization sequence for the synthesis of the dibenzo[b,d]pyran derivs. proved equal or even superior in terms of yield, but is environmentally friendly.  
 IT **374551-18-5P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of dibenzo[b,d]pyrans by oxidation/o-arylation/cyclization of phenols with tris[o-chloromethylphenyl]bismuth diacetate)  
 RN 374551-18-5 CAPLUS  
 CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-11-one, 2,4-dimethoxy- (9CI)  
 (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~LX2~~ ANSWER 15 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:767253 CAPLUS

DOCUMENT NUMBER: 138:205032

TITLE: A photochemical route to dibenzonaphthyrone

AUTHOR(S): Jackson, Yvette A.; Marriott, Karla-Sue C.

CORPORATE SOURCE: Department of Chemistry, University of the West Indies, Kingston, 7, Antigua and Barbuda

SOURCE: Heterocycles (2002), 57(10), 1897-1900

CODEN: HTCYAM; ISSN: 0385-5414

PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:205032

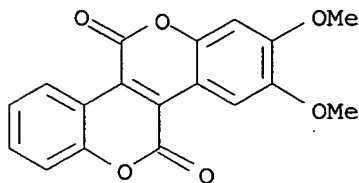
AB 2,3-Dimethoxybenzopyrano[4,3-c]benzopyran-5,11-dione was prepared via photochem. rearrangement of 2-Me 3-Ph 5,6-dimethoxy-1-benzofuran-2,3-dicarboxylate which was synthesized via a multistep route.

IT 500003-10-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and spectra of dimethoxybenzopyranobenzopyrandione from photochem. rearrangement of dimethoxybenzopyranobenzopyrandione)

RN 500003-10-1 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 2,3-dimethoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

10

THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

~~12~~2 ANSWER 16 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:210373 CAPLUS

DOCUMENT NUMBER: 137:87830

TITLE: Molecular simulation of interaction between estrogen receptor and selective estrogen receptor modulators

AUTHOR(S): Guo, Zong-Ru; Yi, Xiang; Xu, Zhi-Bin

CORPORATE SOURCE: Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing, 100050, Peop. Rep. China

SOURCE: Acta Pharmacologica Sinica (2002), 23(3), 208-212  
CODEN: APSCG5; ISSN: 1671-4083

PUBLISHER: Science Press

DOCUMENT TYPE: Journal

LANGUAGE: English

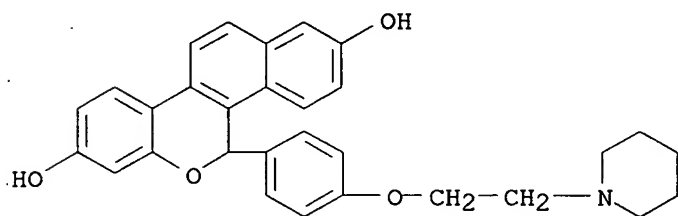
AB Aim: To study the mechanism of interaction between a series of potent racemic selective estrogen receptor modulators (SERM) and estrogen receptors (ER). Methods: Active conformations of these conformationally restricted raloxifene analogs in binding pocket were determined by mol. mechanics. The interactive energies between ligand and receptor were calculated by docking program. Results: Both R and S configurations of these SERM were accommodated by the binding pocket of ER. The hydroxy group of compds. forms hydrogen bonds with amino acid residues of ER and the phenolic group mimics the A-ring of estradiol. The most potential compds. were those with two hydroxy groups and accommodated by binding pocket in S configuration with phenolic group at C(16) imitating A-ring of estradiol. Conclusion: Chiral center conferred little effect on the binding affinity of these conformationally restricted raloxifene analogs. The hydroxy group(s) play(s) a critical role to the orientation of compds. in active pocket of ER and the binding between ligand and receptor.

IT 188824-17-1

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(mol. simulation of estrogen receptor interaction with estrogen receptor modulators)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol, 5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



~~12~~ ANSWER 17 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:557693 CAPLUS

DOCUMENT NUMBER: 135:371601

TITLE: Aryllead triacetates in the synthesis of oxaphenanthrene derivatives

AUTHOR(S): Fedorov, A. Y.; Carrara, F.; Finet, J.-P.

CORPORATE SOURCE: Faculte des Sciences, Biologie et Radicaux Libres, Laboratoire Chimie, UMR 6517, CNRS-Universites d'Aix-Marseille, Saint-Jerome, Marseille, 13397, Fr.

SOURCE: Tetrahedron Letters (2001), 42(34), 5875-5877

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:371601

AB Ortho-Halomethylphenyl-Pb(AcO)<sub>3</sub> (halo = Br, Cl) react with phenols in the presence of NEt<sub>3</sub> and a Py derivative to afford modest to good yields of dibenzo[b,d]-6H-pyrans.

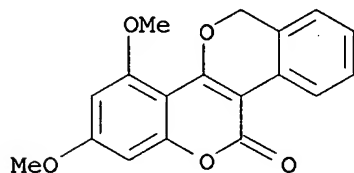
IT 374551-18-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of oxaphenanthrene derivs. by aryllead triacetate-mediated ortho-arylation-cyclization)

RN 374551-18-5 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-11-one, 2,4-dimethoxy- (9CI)  
(CA INDEX NAME)



REFERENCE COUNT:

26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

122 ANSWER 18 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:818588 CAPLUS

DOCUMENT NUMBER: 134:125545

TITLE: Protein-Based Virtual Screening of Chemical Databases.  
1. Evaluation of Different Docking/Scoring  
Combinations

AUTHOR(S): Bissantz, Caterina; Folkers, Gerd; Rognan, Didier

CORPORATE SOURCE: Department of Applied Biosciences, ETH Zuerich,  
Zurich, CH-8057, Switz.SOURCE: Journal of Medicinal Chemistry (2000), 43(25),  
4759-4767

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Three different database docking programs (Dock, FlexX, Gold) have been used in combination with seven scoring functions (Chemscore, Dock, FlexX, Fresno, Gold, Pmf, Score) to assess the accuracy of virtual screening methods against two protein targets (thymidine kinase, estrogen receptor) of known three-dimensional structure. For both targets, it was generally possible to discriminate about 7 out of 10 true hits from a random database of 990 ligands. The use of consensus lists common to two or three scoring functions clearly enhances hit rates among the top 5% scorers from 10% (single scoring) to 25-40% (double scoring) and up to 65-70% (triple scoring). However, in all tested cases, no clear relationships could be found between docking and ranking accuracies. Moreover, predicting the absolute binding free energy of true hits was not possible whatever docking accuracy was achieved and scoring function used. As the best docking/consensus scoring combination varies with the selected target and the physicochem. of target-ligand interactions, we propose a two-step protocol for screening large databases: (i) screening of a reduced dataset containing a few known ligands for deriving the optimal docking/consensus scoring scheme, (ii) applying the latter parameters to the screening of the entire database.

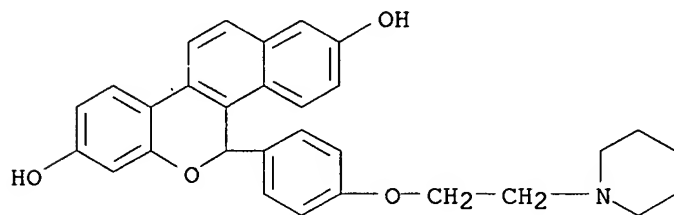
IT 188824-17-1, LY 357489

RL: PRP (Properties)

(accuracy of virtual screening methods against protein targets of known structure)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol, 5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

50

THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/307,735

102 ANSWER 19 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:672817 CAPLUS

DOCUMENT NUMBER: 131:300577

TITLE: Dibenzonaphthyrone, their preparation and use for coloring/pigmenting high-molecular-weight organic material

INVENTOR(S): Nesvadba, Peter; Jandke, Joachim

PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.

SOURCE: PCT Int. Appl., 49 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

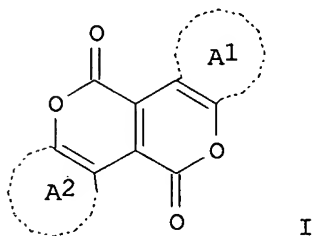
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9952909	A2	19991021	WO 1999-EP2139	19990329
WO 9952909	A3	20000113		
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
AU 9935218	A1	19991101	AU 1999-35218	19990329
BR 9909461	A	20001212	BR 1999-9461	19990329
EP 1095041	A2	20010502	EP 1999-916896	19990329
R:	CH, DE, FR, GB, IT, LI			
US 6281361	B1	20010828	US 1999-280738	19990329
JP 2002511498	T2	20020416	JP 2000-543466	19990329
CN 1125072	B	20031022	CN 1999-804890	19990329
US 2002095046	A1	20020718	US 2001-880211	20010613
US 6533825	B2	20030318		
PRIORITY APPLN. INFO.:			CH 1998-838	A 19980408
			CH 1998-1861	A 19980911
			US 1999-280738	A3 19990329
			WO 1999-EP2139	W 19990329

OTHER SOURCE(S): MARPAT 131:300577

GI



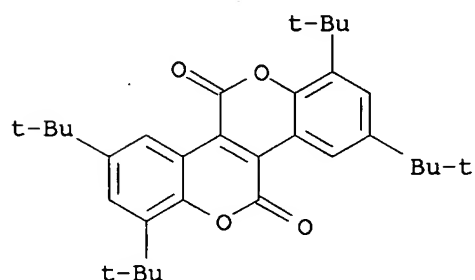
AB Dibenzonaphthyrone I (A1, A2 = C6-18 aromatic system bearing 0-4 substituents), exclusive of 14 specific known compds., are claimed; all the I are useful for bulk coloration of plastics. Thus, 2,4-di-tert-butylphenol (II) was cyclocondensed with glyoxylic acid to give 5,7-di-tert-butyl-3-hydroxybenzofuran-2(3H)-one, which was thermally dehydratively dimerized to the isoxindigo in 76% yield (based on II) and further heated in refluxing BuOH containing pyridine for 16 h to give 95% 1,3,7,9-tetra-tert-butyl[1]benzopyrano[4,3-c][1]benzopyran-5,11-dione, which showed high lightfastness and color intensity in PET and PBT.

IT 80360-50-5P 80360-51-6P 80360-52-7P  
247128-93-4P 247128-94-5P 247128-95-6P  
247128-96-7P 247128-97-8P 247128-98-9P  
247128-99-0P 247129-00-6P 247129-01-7P  
247129-02-8P

RL: MOA (Modifier or additive use); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)  
(preparation of dibenzonaphthyrone for coloring high-mol.-weight organic material)

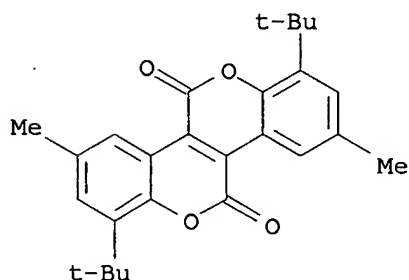
RN 80360-50-5 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 1,3,7,9-tetrakis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



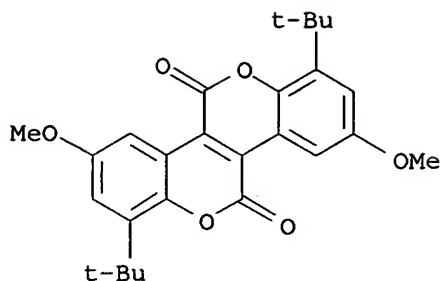
RN 80360-51-6 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 1,7-bis(1,1-dimethylethyl)-3,9-dimethyl- (9CI) (CA INDEX NAME)

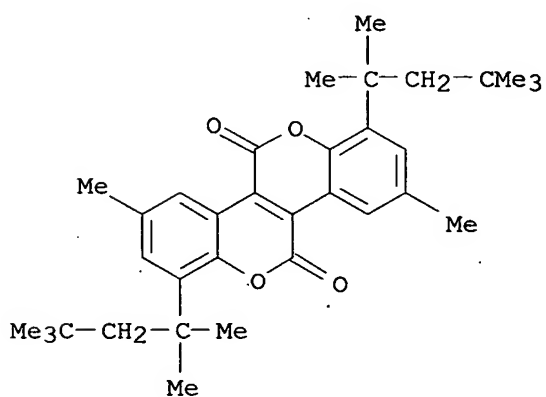


RN 80360-52-7 CAPLUS

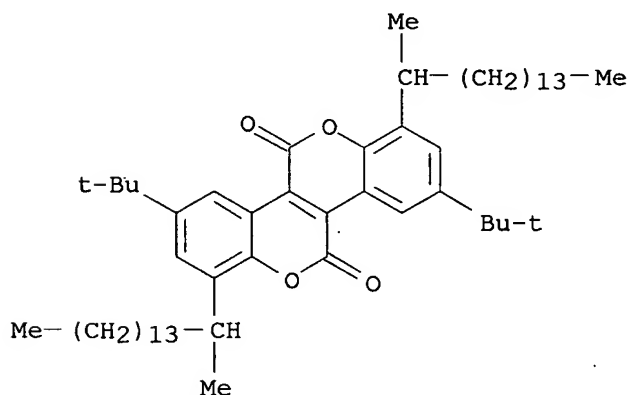
CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 1,7-bis(1,1-dimethylethyl)-3,9-dimethoxy- (9CI) (CA INDEX NAME)



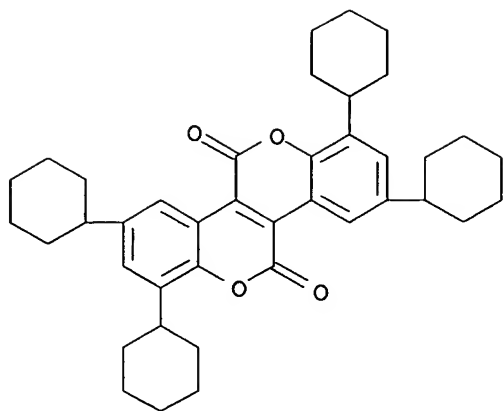
RN 247128-93-4 CAPLUS  
CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 3,9-dimethyl-1,7-bis(1,1,3,3-tetramethylbutyl)- (9CI) (CA INDEX NAME)



RN 247128-94-5 CAPLUS  
CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 3,9-bis(1,1-dimethylethyl)-  
1,7-bis(1-methylpentadecyl)- (9CI) (CA INDEX NAME)

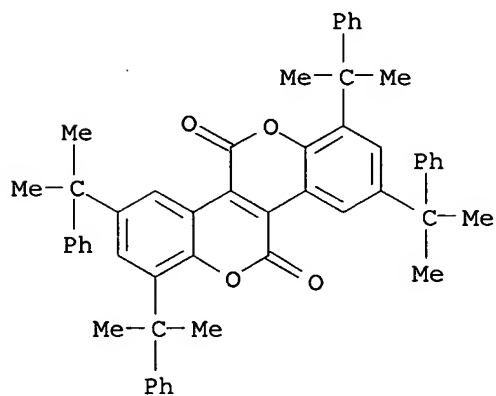


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RN      247128-95-6  CAPLUS
CN      [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 1,3,7,9-tetracyclohexyl-
        (9CI)  (CA INDEX NAME)
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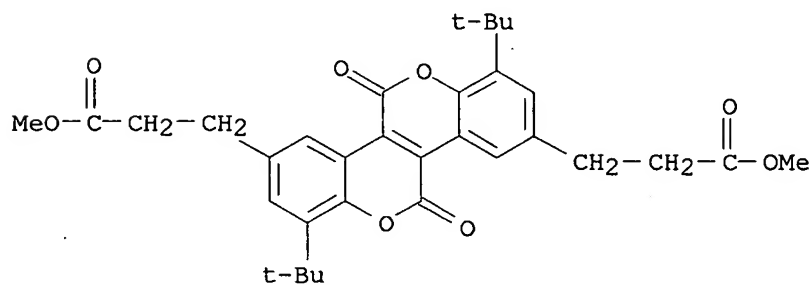
RN 247128-96-7 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 1,3,7,9-tetrakis(1-methyl-1-phenylethyl)- (9CI) (CA INDEX NAME)



RN 247128-97-8 CAPLUS

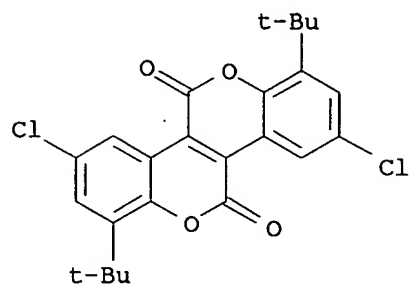
CN [1]Benzopyrano[4,3-c][1]benzopyran-3,9-dipropanoic acid, 1,7-bis(1,1-dimethylethyl)-5,11-dihydro-5,11-dioxo-, dimethyl ester (9CI) (CA INDEX NAME)



RN 247128-98-9 CAPLUS

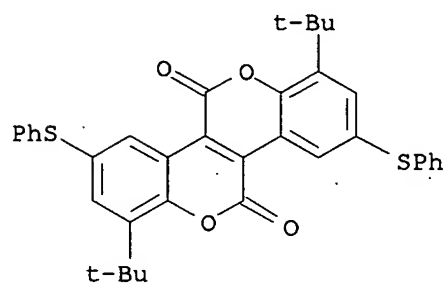
10/307,735

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 3,9-dichloro-1,7-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



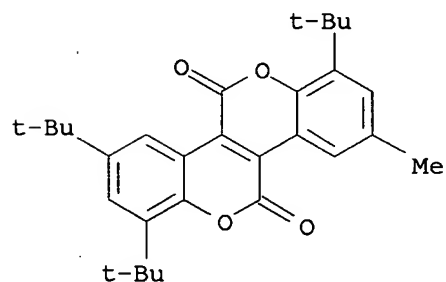
RN 247128-99-0 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 1,7-bis(1,1-dimethylethyl)-3,9-bis(phenylthio)- (9CI) (CA INDEX NAME)



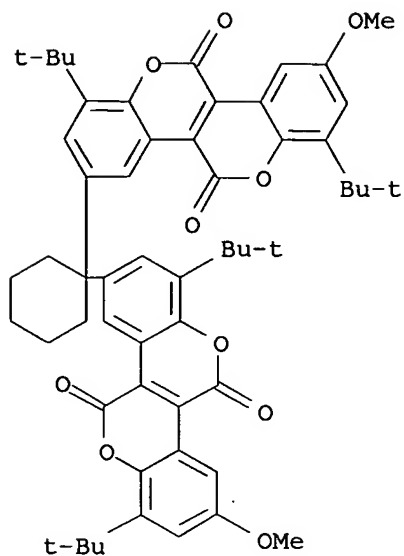
RN 247129-00-6 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 1,3,7-tris(1,1-dimethylethyl)-9-methyl- (9CI) (CA INDEX NAME)



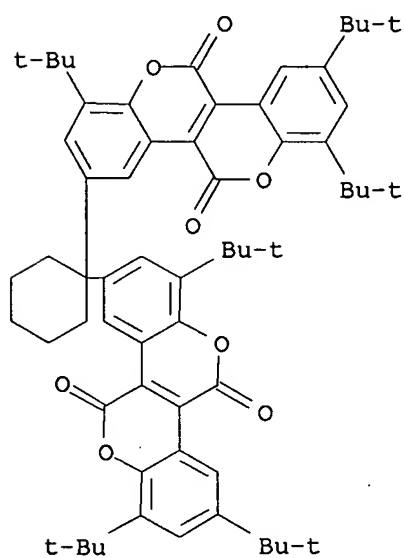
RN 247129-01-7 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 3,3'-cyclohexylidenebis[1,7-bis(1,1-dimethylethyl)-9-methoxy- (9CI) (CA INDEX NAME)



RN 247129-02-8 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 3,3'-  
cyclohexylidenebis[1,7,9-tris(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)





~~122~~ ANSWER 20 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:480561 CAPLUS

DOCUMENT NUMBER: 131:170255

TITLE: A new method for the synthesis of 1/3-substituted-6H-[2]-benzopyrano[4,3-c]quinoline-6,11-[12H]-diones and [2] benzopyrano-[4,3-c][1]benzopyran-5,12-diones

AUTHOR(S): Mulwad, V. V.; Lohar, M. V.

CORPORATE SOURCE: Department of Chemistry, The Institute of Science, Mumbai, 400 032, India

SOURCE: Indian Journal of Heterocyclic Chemistry (1999), 8(4), 337-338

CODEN: IJCHEI; ISSN: 0971-1627

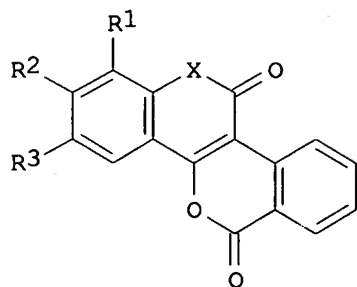
PUBLISHER: Prof. R. S. Varma

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 131:170255

GI



I

AB A new and facile method for the synthesis of 1/3-substituted-6H-[2]-benzopyrano[4,3-c]quinoline-6,11-[12H]-diones and [2]benzopyrano[4,3-c][1]benzopyran-5,12-diones I (R1 = H, Me, OMe, Ph, 4-MeC6H4, Et; R2 = H, Me; R3 = H, Me, OMe, Cl, Br; X = NH, NR1, O) by the condensation of 4-hydroxy-2-quinolones or 4-hydroxycoumarins with Me salicylate has been developed. This method offers better yields as compared to previously known methods.

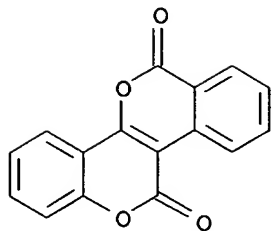
IT 2288-98-4P 27284-76-0P 27284-78-2P  
27284-80-6P 238751-25-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

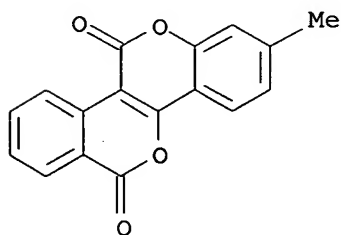
(preparation of benzopyranoquinolinediones and benzopyranobenzopyrandiones via cyclocondensation of hydroxyquinolines or hydroxycoumarins and Me salicylate)

RN 2288-98-4 CAPLUS

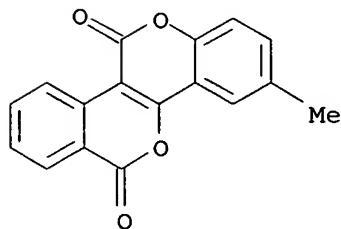
CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione (8CI, 9CI) (CA INDEX NAME)



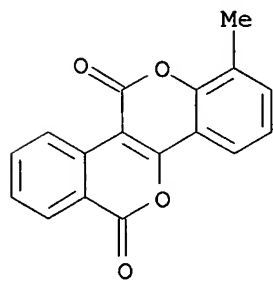
RN 27284-76-0 CAPLUS  
 CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 2-methyl- (8CI, 9CI)  
 (CA INDEX NAME)



RN 27284-78-2 CAPLUS  
 CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 3-methyl- (8CI, 9CI)  
 (CA INDEX NAME)



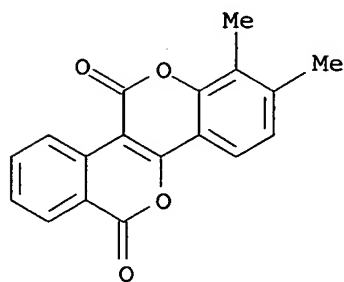
RN 27284-80-6 CAPLUS  
 CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 1-methyl- (8CI, 9CI)  
 (CA INDEX NAME)



10/307,735

RN 238751-25-2 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 1,2-dimethyl- (9CI)  
(CA INDEX NAME)



REFERENCE COUNT:

5

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

122 ANSWER 21 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:215077 CAPLUS

DOCUMENT NUMBER: 128:266187

TITLE: Synthesis and Pharmacology of Conformationally Restricted Raloxifene Analogs: Highly Potent Selective Estrogen Receptor Modulators

AUTHOR(S): Grese, Timothy A.; Pennington, Lewis D.; Sluka, James P.; Adrian, M. Dee; Cole, Harlan W.; Fuson, Tina R.; Magee, David E.; Phillips, D. Lynn; Rowley, Ellen R.; Shetler, Pamela K.; Short, Lorri L.; Venugopalan, Murali; Yang, Na N.; Sato, Masahiko; Glasebrook, Andrew L.; Bryant, Henry U.

CORPORATE SOURCE: Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, IN, 46285, USA

SOURCE: Journal of Medicinal Chemistry (1998), 41(8), 1272-1283

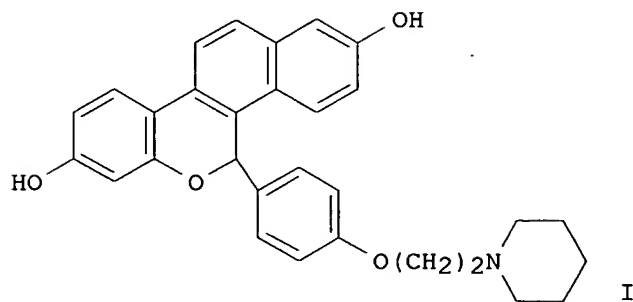
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Raloxifene is a selective estrogen receptor modulator (SERM) which is currently under clin. evaluation for the prevention and treatment of postmenopausal osteoporosis. In vivo structure-activity relationships and mol. modeling studies indicated that the orientation of the basic amine-containing side chain of raloxifene relative to the stilbene plane is an important discriminating factor for the maintenance of tissue selectivity. A series of raloxifene analogs where this side chain is held in an orientation which is orthogonal to the stilbene plane, similar to the low-energy conformation predicted for raloxifene were constructed. These analogs were prepared and tested for their activity in a series of in vitro and in vivo biol. assays reflective of the SERM profile. The ability of these analogs to (1) bind the estrogen receptor, (2) antagonize estrogen-stimulated proliferation of MCF-7 cells in vitro, (3) stimulate TGF- $\beta$ 3 gene expression in cell culture, (4) inhibit the uterine effects of ethynyl estradiol in immature rats, and (5) potentially reduce serum cholesterol and protect against osteopenia in ovariectomized (OVX) rats without estrogen-like stimulation of uterine tissue is detailed. These data demonstrate that LY357489 (I) is among the most potent SERMs described to date with in vivo efficacy on bone and cholesterol metabolism in OVX rats at doses as low as 0.01 mg/kg/d.

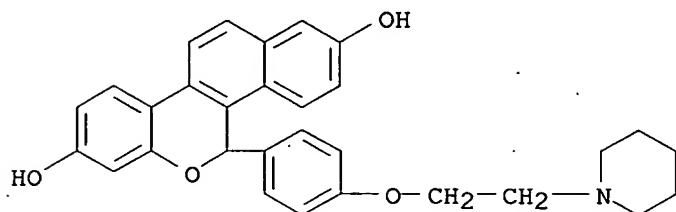
IT 188824-17-1P, LY 357489

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of conformationally restricted raloxifene analogs and pharmacol. as selective estrogen receptor modulators)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol, 5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



IT 188824-49-9P 188824-50-2P 188824-51-3P

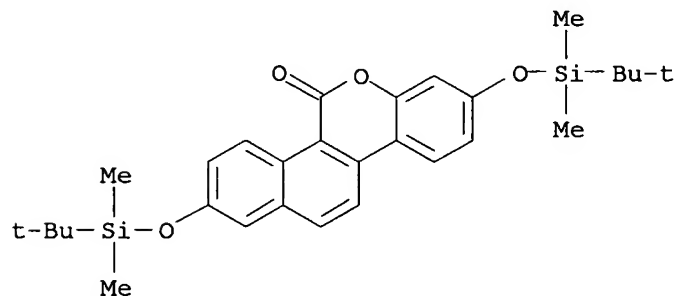
188824-59-1P 204141-62-8P 205318-98-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of conformationally restricted raloxifene analogs and pharmacol. as selective estrogen receptor modulators)

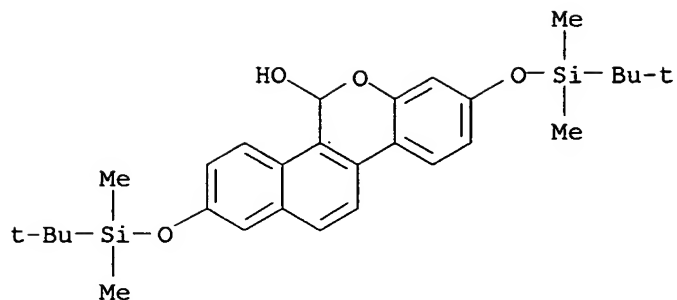
RN 188824-49-9 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-5-one, 2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]- (9CI) (CA INDEX NAME)



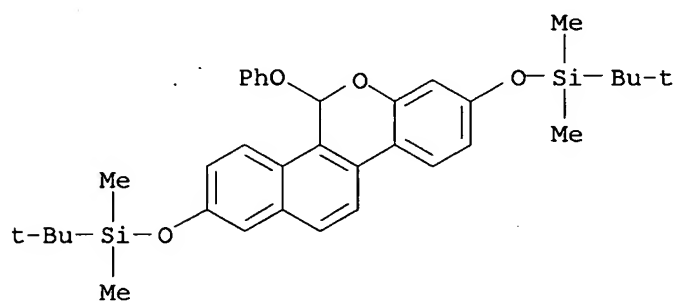
RN 188824-50-2 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-5-ol, 2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]- (9CI) (CA INDEX NAME)



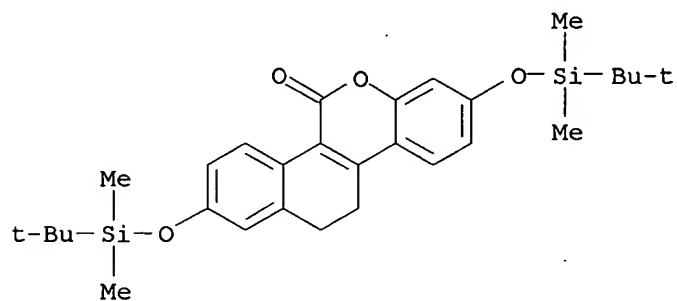
RN 188824-51-3 CAPLUS

CN Silane, [(5-phenoxy-5H-benzo[b]naphtho[2,1-d]pyran-2,8-diyl)bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



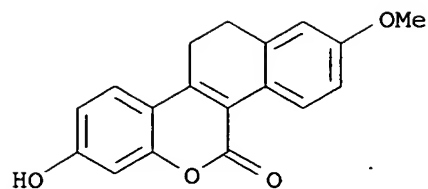
RN 188824-59-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-5-one, 2,8-bis[(1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro- (9CI) (CA INDEX NAME)



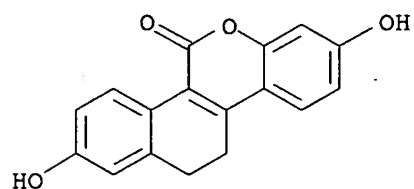
RN 204141-62-8 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-5-one, 11,12-dihydro-8-hydroxy-2-methoxy- (9CI) (CA INDEX NAME)



RN 205318-98-5 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-5-one, 11,12-dihydro-2,8-dihydroxy- (9CI)  
(CA INDEX NAME)



REFERENCE COUNT:

60

THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 22 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:180547 CAPLUS

DOCUMENT NUMBER: 128:217362

TITLE: Preparation of benzothienobenzopyrans, benzophenanthridines, and related compounds for treatment of postmenopausal syndrome.

INVENTOR(S): Grese, Timothy Alan

PATENT ASSIGNEE(S): Eli Lilly and Co., USA

SOURCE: U.S., 39 pp.  
CODEN: USXXAM

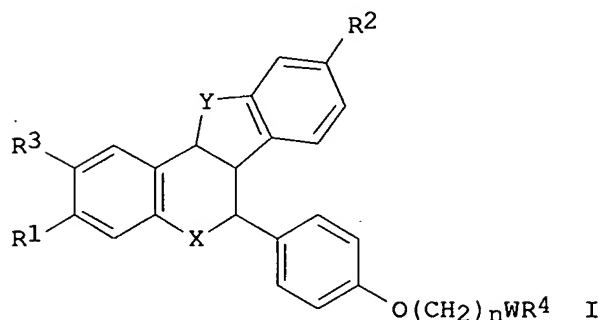
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5726186	A	19980310	US 1996-696279	19960813
US 6004971	A	19991221	US 1997-878799	19970619
US 6133288	A	20001017	US 1999-436743	19991109
PRIORITY APPLN. INFO.:			US 1995-3496P	P 19950908
			US 1996-696279	A3 19960813
			US 1997-878799	A1 19970619

OTHER SOURCE(S): MARPAT 128:217362  
GI

AB Title compds. [I; X = O, S; Y = O, S, CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>, CH:CH, NR<sub>5</sub>; R<sub>1</sub>-R<sub>3</sub> = H, OH, alkoxy, PhCO<sub>2</sub>, alkylcarbonyloxy, alkylsulfonyloxy, OSO<sub>2</sub>CF<sub>3</sub>, Cl, F; n = 1, 2; W = CH<sub>2</sub>, CO; R<sub>4</sub> = 1-piperidinyl, 2-oxo-1-piperidinyl, 1-pyrrolidinyl, methyl-1-pyrrolidinyl, dimethyl-1-pyrrolidinyl, 2-oxo-1-pyrrolidinyl, 4-morpholino, dimethylamino, diethylamino, 1-hexamethyleneimino; R<sub>5</sub> = alkyl, PhCO, alkylcarbonyl, phenoxycarbonyl, alkoxycarbonyl, alkylsulfonyl, phenylsulfonyl, SO<sub>2</sub>CF<sub>3</sub>], were prepared. Thus, 6-methoxythianaphthalen-2-one (preparation given) was stirred with 4-methoxysalicylaldehyde and Et<sub>3</sub>N in CH<sub>2</sub>Cl<sub>2</sub> to give 6a, 11a-dihydro-3,9-dimethoxy-6H-[1]benzothieno[3,2-c][1]benzopyran-6-one. This was converted in several steps to 3,9-dihydroxy-6-[4-[2-(1-piperidinyl)ethoxy]phenyl]-6H-[1]benzothieno[3,2-c][1]benzopyran. The latter at 0.1 mg/kg in ovariectomized rats reduced serum cholesterol by 72.8%.

IT 188824-17-1P

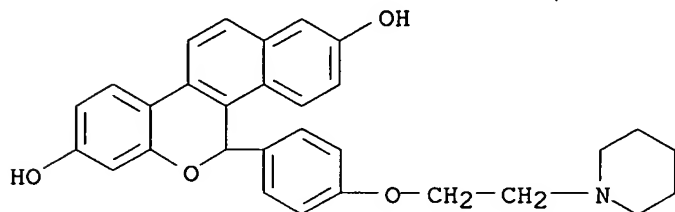
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)



(preparation of benzothienobenzopyrans, benzophenanthridines, and related compds. for treatment of postmenopausal syndrome)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol, 5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



IT 188824-49-9P 188824-50-2P 188824-51-3P

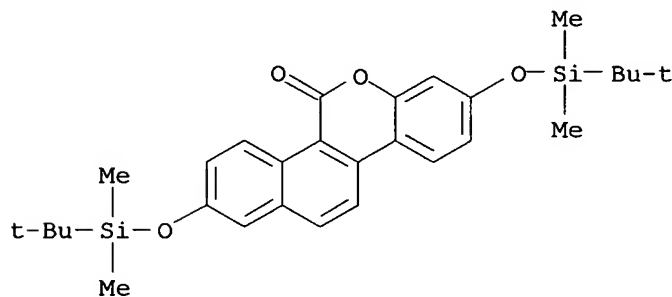
188824-52-4P 188824-59-1P 204141-62-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of benzothienobenzopyrans, benzophenanthridines, and related compds. for treatment of postmenopausal syndrome)

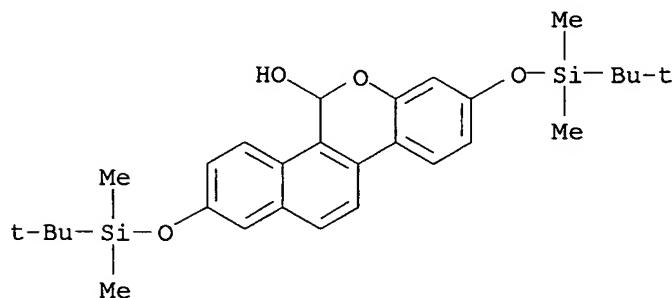
RN 188824-49-9 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-5-one, 2,8-bis[[1,1-dimethylethyl)dimethylsilyl]oxy]- (9CI) (CA INDEX NAME)



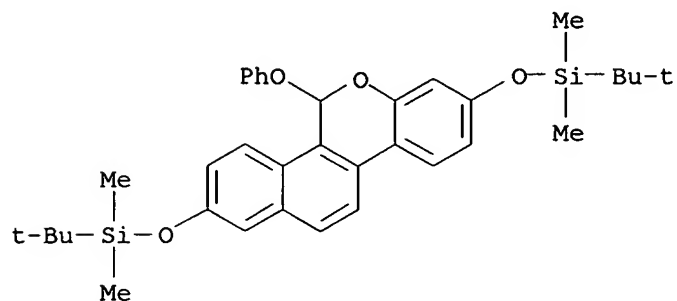
RN 188824-50-2 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-5-ol, 2,8-bis[[1,1-dimethylethyl)dimethylsilyl]oxy]- (9CI) (CA INDEX NAME)



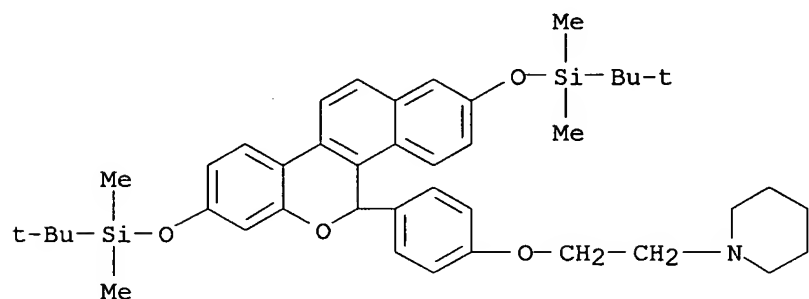
RN 188824-51-3 CAPLUS

CN Silane, [(5-phenoxy-5H-benzo[b]naphtho[2,1-d]pyran-2,8-diyl)bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



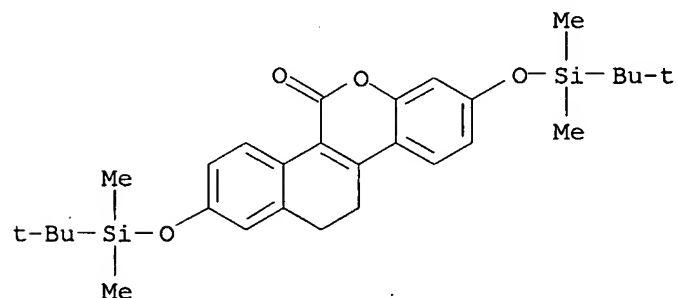
RN 188824-52-4 CAPLUS

CN Piperidine, 1-[2-[4-[2,8-bis[[ (1,1-dimethylethyl)dimethylsilyl]oxy]-5H-benzo[b]naphtho[2,1-d]pyran-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



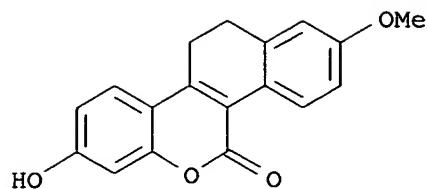
RN 188824-59-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-5-one, 2,8-bis[[ (1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro- (9CI) (CA INDEX NAME)



RN 204141-62-8 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-5-one, 11,12-dihydro-8-hydroxy-2-methoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

9

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/307,735

~~L72~~ ANSWER 23 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:286346 CAPLUS

DOCUMENT NUMBER: 126:264018

TITLE: Preparation of pentacyclic compounds for the treatment conditions associated with post-menopausal syndrome

INVENTOR(S): Grese, Timothy Alan

PATENT ASSIGNEE(S): Eli Lilly and Co., USA

SOURCE: Eur. Pat. Appl., 72 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 761669	A2	19970312	EP 1996-306351	19960902
EP 761669	A3	19971029		
EP 761669	B1	20001122		
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
CA 2230974	AA	19970313	CA 1996-2230974	19960826
WO 9709044	A1	19970313	WO 1996-US13778	19960826
W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9669590	A1	19970327	AU 1996-69590	19960826
AU 705454	B2	19990520		
CN 1201392	A	19981209	CN 1996-198083	19960826
BR 9610356	A	19990706	BR 1996-10356	19960826
JP 11514347	T2	19991207	JP 1996-511257	19960826
CZ 286236	B6	20000216	CZ 1998-678	19960826
IL 123560	A1	20020210	IL 1996-123560	19960826
IL 140162	A1	20020210	IL 1996-140162	19960826
AT 197712	E	20001215	AT 1996-306351	19960902
NO 9800936	A	19980507	NO 1998-936	19980304
GR 3035253	T3	20010430	GR 2001-400073	20010117
PRIORITY APPLN. INFO.:			US 1995-3496P	P 19950908
			IL 1996-123560	A3 19960826
			WO 1996-US13778	W 19960826

OTHER SOURCE(S): MARPAT 126:264018

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The title compds. [I and II; X = O, S, NR5 (wherein R5 = C1-3 alkyl, CPh, SO2CF3, etc.); Y = O, S, CH2, CH2CH2, CH:CH, NR5; B = CH2, CO; R1-R3 = H, OH, O(C1-C4 alkyl), etc.; n = 1, 2; W = CH2, CO; R4 = 1-piperidinyl, 2-oxo-1-piperidinyl, 1-pyrrolidinyl, etc.], useful for the treatment of the various conditions associated with post-menopausal syndrome such as osteoporosis, and uterine fibroid disease, endometriosis, and aortal smooth muscle cell proliferation, and as bone loss or resorption inhibitors and serum cholesterol levels lowering agents, were prepared and

formulated. Thus, reaction of 3,9-bis[(tert-butyl dimethylsilyl)oxy]-6-phenox-6-H-[1]benzothieno[3,2-c][1]benzopyran with 4-(2-piperidinoethoxy)phenylmagnesium bromide in PhMe/THF followed by removal of TBDMS groups with TBAF in THF afforded III which showed IC<sub>50</sub> of 0.2 nM against MCF-7 breast adenocarcinoma cells proliferation.

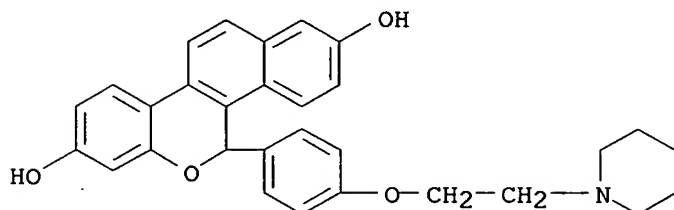
IT 188824-17-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pentacyclic compds. for the treatment conditions associated with post-menopausal syndrome)

RN 188824-17-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-2,8-diol, 5-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



IT 188824-49-9P 188824-50-2P 188824-51-3P

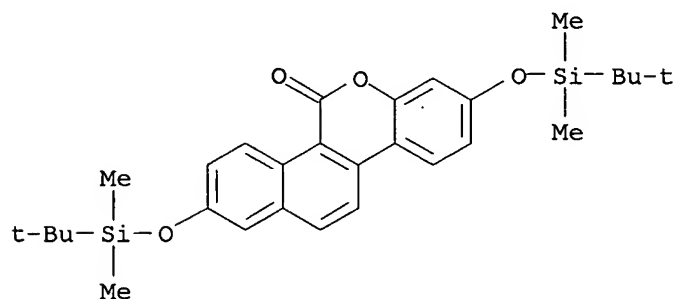
188824-52-4P 188824-58-0P 188824-59-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pentacyclic compds. for the treatment conditions associated with post-menopausal syndrome)

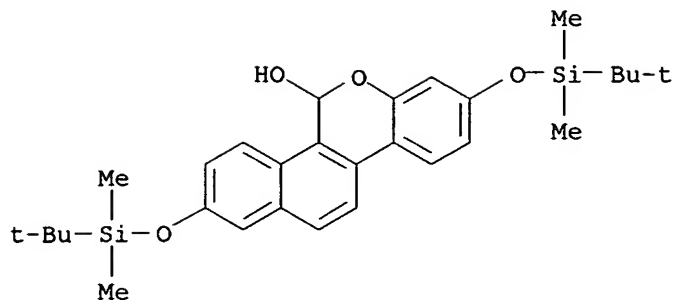
RN 188824-49-9 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-5-one, 2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]- (9CI) (CA INDEX NAME)



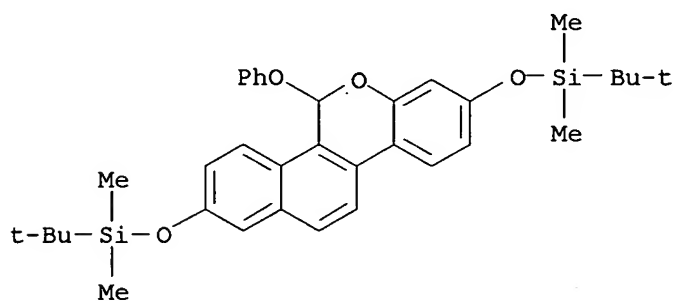
RN 188824-50-2 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-5-ol, 2,8-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]- (9CI) (CA INDEX NAME)



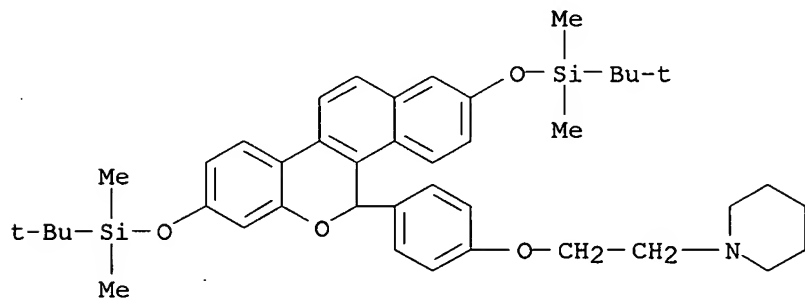
RN 188824-51-3 CAPLUS

CN Silane, [(5-phenoxy-5H-benzo[b]naphtho[2,1-d]pyran-2,8-diyl)bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



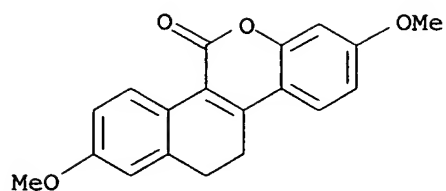
RN 188824-52-4 CAPLUS

CN Piperidine, 1-[2-[4-[2,8-bis[[ (1,1-dimethylethyl)dimethylsilyl]oxy]-5H-benzo[b]naphtho[2,1-d]pyran-5-yl]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



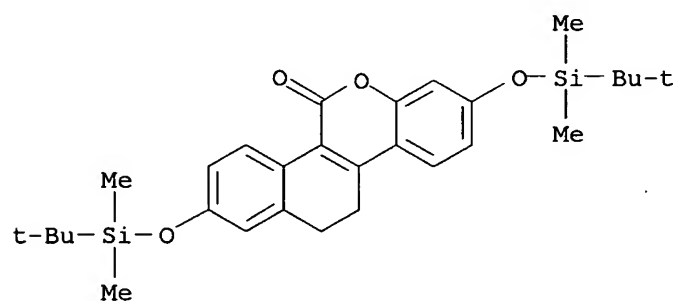
RN 188824-58-0 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-5-one, 11,12-dihydro-2,8-dimethoxy- (9CI) (CA INDEX NAME)



RN 188824-59-1 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-5-one, 2,8-bis[[ (1,1-dimethylethyl)dimethylsilyl]oxy]-11,12-dihydro- (9CI) (CA INDEX NAME)



L22 ANSWER 24 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:469268 CAPLUS

DOCUMENT NUMBER: 123:285826

TITLE: Reactions with 2(1H)-quinolinone and coumarin derivatives: new routes to polysubstituted 2(1H)-quinolinone and coumarin derivatives

AUTHOR(S): El-Taweel, Fathy Mohamed Abdel Aziz; Zaki, Salah; Sowellim, Ahmed; Elagamey, Abdel Ghani Ali

CORPORATE SOURCE: Dep. Chemistry, Faculty Science, New Damietta University, Egypt

SOURCE: Bulletin of the Chemical Society of Japan (1995), 68(3), 905-10

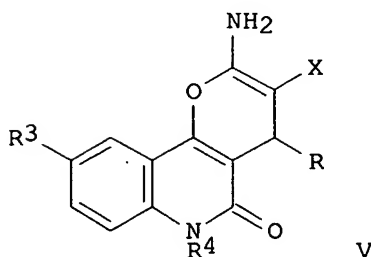
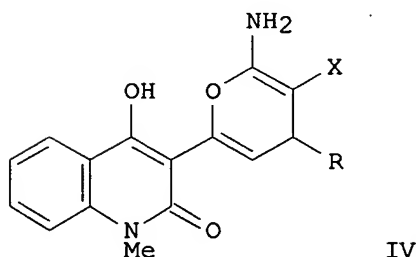
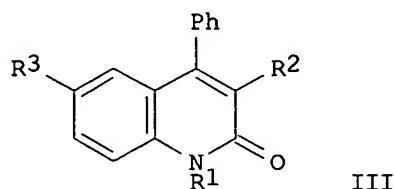
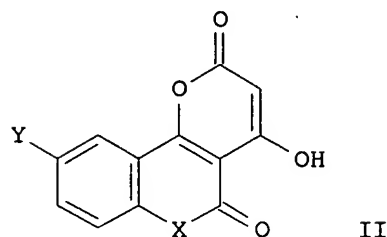
CODEN: BCSJA8; ISSN: 0009-2673

PUBLISHER: Nippon Kagakkai

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Whereas reaction of benzylidenenitriles  $RCH:C(CN)X_1$  [I, R = Ph, 4-MeOC<sub>6</sub>H<sub>4</sub>, 4-ClC<sub>6</sub>H<sub>4</sub>; X<sub>1</sub> = CN, CO<sub>2</sub>Et] (or a mixture of either malononitrile or Et cyanoacetate and aromatic aldehydes) with pyranoquinolinedione II (X = NMe, Y = H) or quinolinone III (R<sub>1</sub> = Me, R<sub>2</sub> = Ac, R<sub>3</sub> = H) in ethanol/piperidine gave 4H-pyran derivs. IV, the reaction of II (X = NEt, Y = H; X = NH, Y = Cl) or III (R<sub>1</sub> = Et, R<sub>2</sub> = Ac, R<sub>3</sub> = H; R<sub>1</sub> = H, R<sub>2</sub> = Ac, R<sub>3</sub> = Cl) with the same reagents afforded pyranoquinolinones V (R<sub>4</sub> = Et, H). V (R<sub>4</sub> = Et, H) were also prepared from I and III (R<sub>1</sub> = Et, R<sub>2</sub> = R<sub>3</sub> = H; R<sub>1</sub> = R<sub>2</sub> = H, R<sub>3</sub> = Cl; R<sub>1</sub> = Et, R<sub>2</sub> = CHO, R<sub>3</sub> = Cl). Reaction of pyranocoumarin II (X = O, Y = H) with I (R = Ph, X<sub>1</sub> = CN) yielded a benzopyranobenzopyran-6,11-dione derivative. Treatment of bromide III (R<sub>1</sub> = Et, R<sub>2</sub> = COCH<sub>2</sub>Br, R<sub>3</sub> = H) with

aqueous

KCN or hydroxylamine afforded the substitution derivative III (R<sub>1</sub> = Et, R<sub>2</sub> = COCH<sub>2</sub>CONH<sub>2</sub>, R<sub>3</sub> = H) and oxime III [R<sub>1</sub> = Et, R<sub>2</sub> = C(CH<sub>2</sub>Br):NOH, R<sub>3</sub> = H] resp.

IT 169308-32-1P

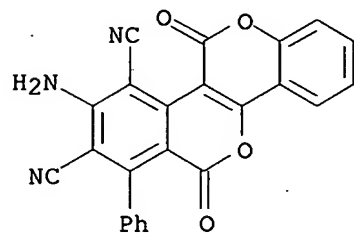


10/307,735

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of pyrans and pyranoquinolinones)

RN 169308-32-1 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-8,10-dicarbonitrile,  
9-amino-6,11-dioxo-7-phenyl- (9CI) (CA INDEX NAME)



L72 ANSWER 25 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:591276 CAPLUS

DOCUMENT NUMBER: 121:191276

TITLE: Electrophotographic photoreceptors using novel bisazo-type carrier-generating agent

INVENTOR(S): Shibata, Toyoko; Fujimoto, Shingo

PATENT ASSIGNEE(S): Konishiroku Photo Ind, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 24 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

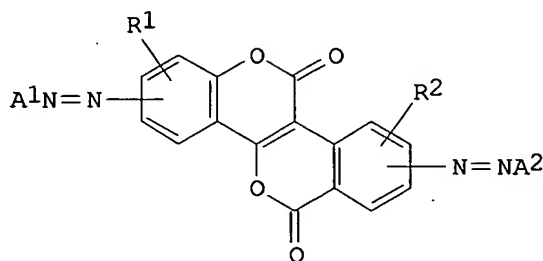
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

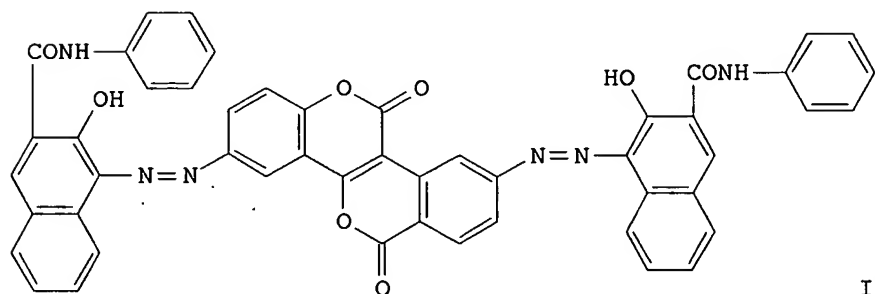
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06110233	A2	19940422	JP 1992-258472	19920928
PRIORITY APPLN. INFO.:			JP 1992-258472	19920928
OTHER SOURCE(S):	MARPAT	121:191276		

GI



I



II

AB The photoreceptors comprise a conductive support with a coating of a photoreceptor layer containing an bisazo compound I [R1, R2 = H, halo, lower alkyl, lower alkoxy, CN; A1, A2 = coupler residue with OH group having coupling ability]. The photoreceptors show high photosensitivity, low residual potential, and good durability in repeated use, and the compound exhibits good carrier-generating properties in combinations with any type of carrier-transporting agents. Thus, an A1 vapor-deposited polyester film with an interlayer was coated with a carrier-generating layer containing II and with a carrier-transporting layer containing a stilbene compound to give a photoreceptor.

IT 157687-27-9 157687-28-0 157687-29-1  
157687-30-4 157687-31-5 157687-32-6

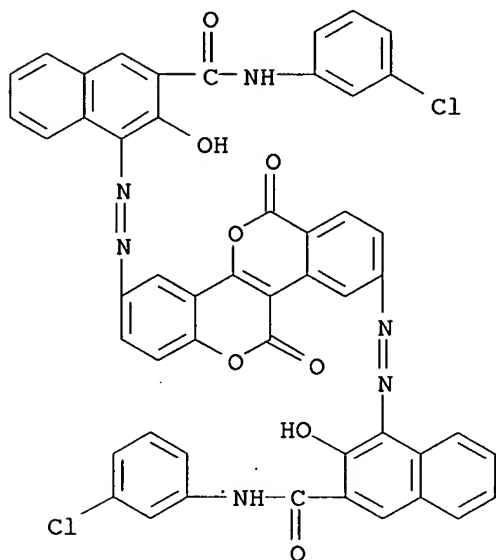
157687-33-7 157687-34-8 157687-35-9  
 157687-36-0 157687-37-1 157687-38-2  
 157687-39-3 157687-40-6 157687-41-7  
 157959-55-2 157959-56-3 157959-57-4  
 157959-58-5 157959-59-6

RL: USES (Uses)

(carrier-generating agent, electrophotog. photoreceptor using)

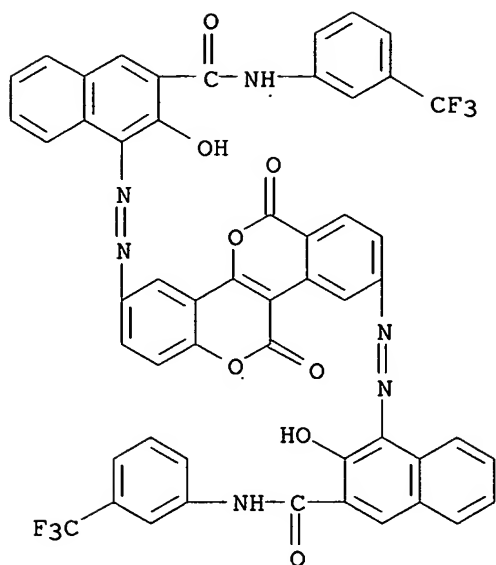
RN 157687-27-9 CAPLUS

CN 2-Naphthalenecarboxamide, 4,4'-[(6,11-dioxo-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-3,9-diyl)bis(azo)]bis[N-(3-chlorophenyl)-3-hydroxy- (9CI)  
 (CA INDEX NAME)



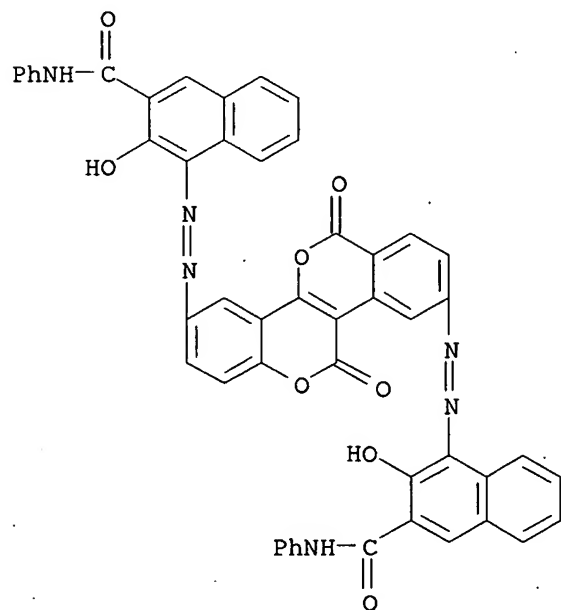
RN 157687-28-0 CAPLUS

CN 2-Naphthalenecarboxamide, 4,4'-[(6,11-dioxo-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-3,9-diyl)bis(azo)]bis[3-hydroxy-N-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



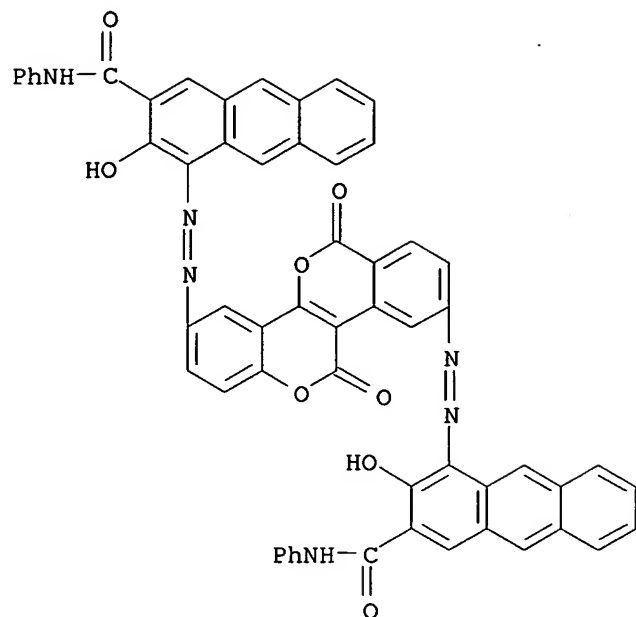
RN 157687-29-1 CAPLUS

CN 2-Naphthalenecarboxamide, 4,4'-[(6,11-dioxo-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-3,9-diyl)bis(azo)]bis[3-hydroxy-N-phenyl- (9CI) (CA INDEX NAME)



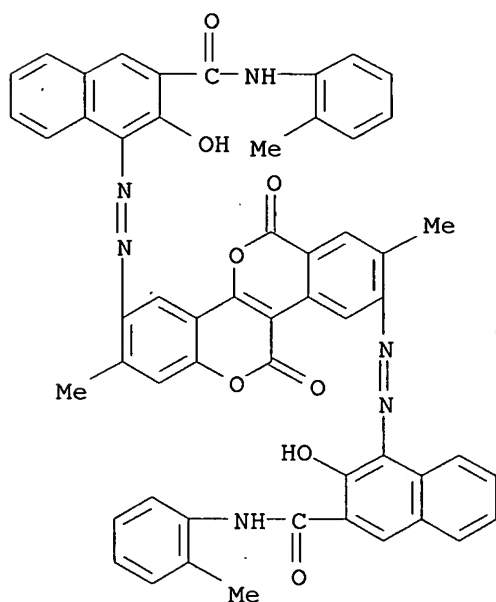
RN 157687-30-4 CAPLUS

CN 2-Anthracenecarboxamide, 4,4'-[(6,11-dioxo-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-3,9-diyl)bis(azo)]bis[3-hydroxy-N-phenyl- (9CI) (CA INDEX NAME)



RN 157687-31-5 CAPLUS

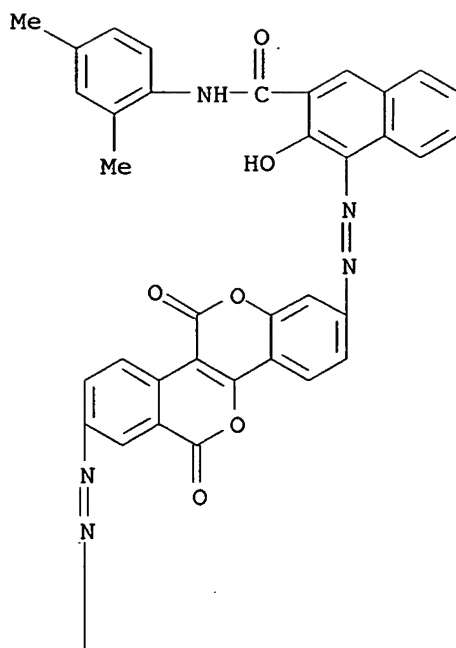
CN 2-Naphthalenecarboxamide, 4,4'-[(2,8-dimethyl-6,11-dioxo-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-3,9-diyl)bis(azo)]bis[3-hydroxy-N-(2-methylphenyl)- (9CI) (CA INDEX NAME)



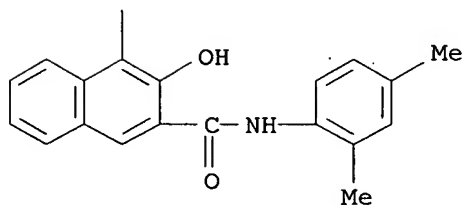
RN 157687-32-6 CAPLUS

CN 2-Naphthalenecarboxamide, 4,4'-[(6,11-dioxo-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-2,8-diyl)bis(azo)]bis[N-(2,4-dimethylphenyl)-3-hydroxy- (9CI) (CA INDEX NAME)

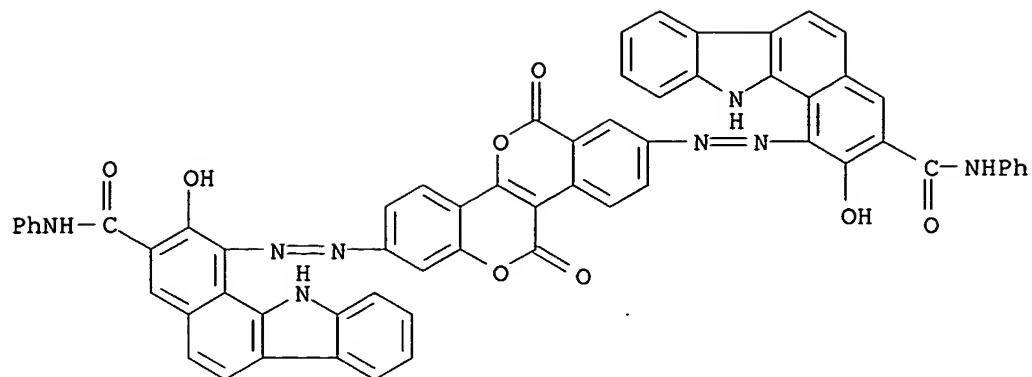
PAGE 1-A



PAGE 2-A



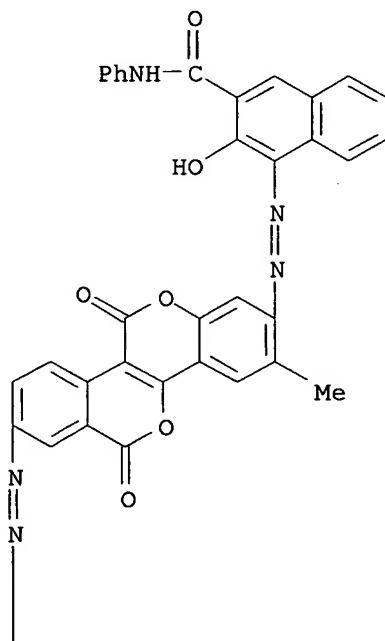
RN 157687-33-7 CAPLUS  
 CN 11H-Benzo[a]carbazole-3-carboxamide, 1,1'-[(6,11-dioxo-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-2,8-diyl)bis(azo)]bis[2-hydroxy-N-phenyl- (9CI) (CA INDEX NAME)



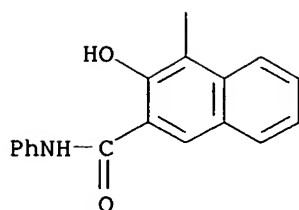
RN 157687-34-8 CAPLUS

CN 2-Naphthalenecarboxamide, 4,4'-[(3-methyl-6,11-dioxo-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-2,8-diyl)bis(azo)]bis[3-hydroxy-N-phenyl- (9CI) (CA INDEX NAME)

PAGE 1-A

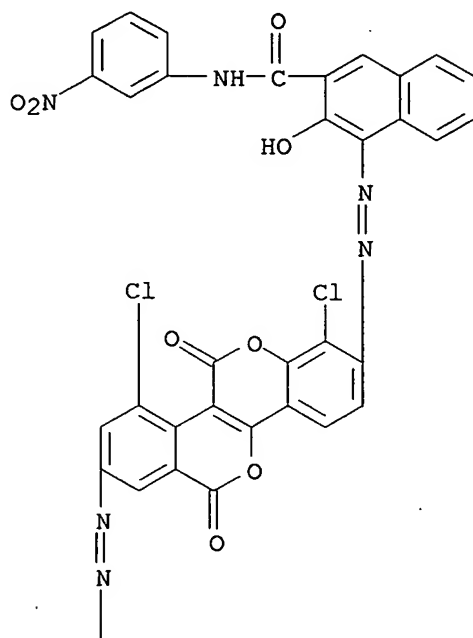


PAGE 2-A

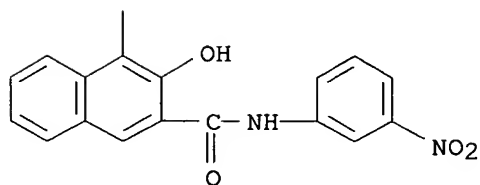


RN 157687-35-9 CAPLUS  
 CN 2-Naphthalenecarboxamide, 4,4'-[(1,10-dichloro-6,11-dioxo-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-2,8-diyl)bis(azo)]bis[3-hydroxy-N-(3-nitrophenyl)-(9CI) (CA INDEX NAME)

PAGE 1-A



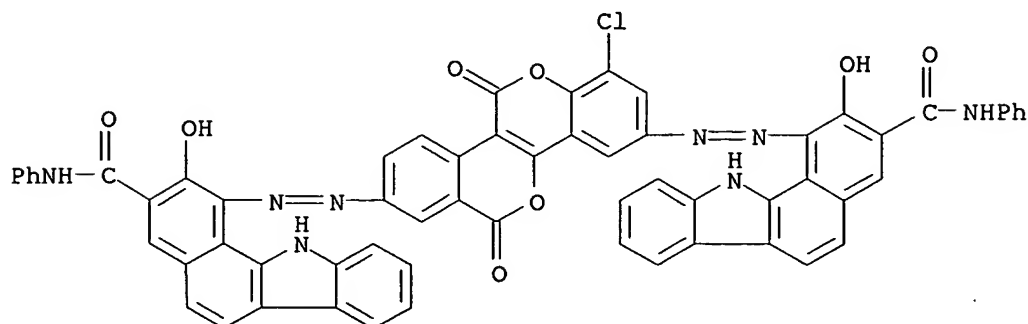
PAGE 2-A



RN 157687-36-0 CAPLUS  
 CN 11H-Benzo[a]carbazole-3-carboxamide, 1,1'-[(1-chloro-6,11-dioxo-6H,11H-

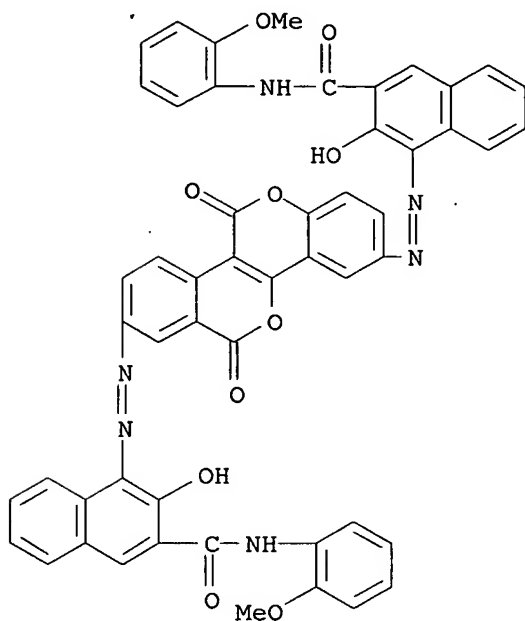


[2]benzopyrano[4,3-c][1]benzopyran-2,8-diyl)bis(azo)]bis[2-hydroxy-N-phenyl- (9CI) (CA INDEX NAME)



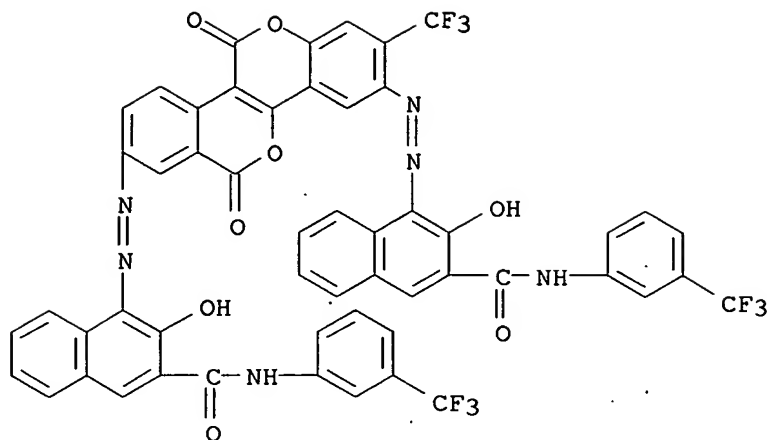
RN 157687-37-1 CAPLUS

CN 2-Naphthalenecarboxamide, 4,4'-[(6,11-dioxo-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-3,8-diyl)bis(azo)]bis[3-hydroxy-N-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



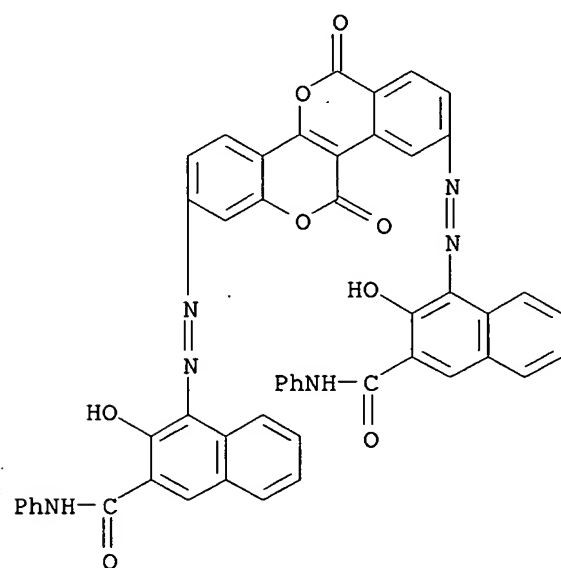
RN 157687-38-2 CAPLUS

CN 2-Naphthalenecarboxamide, 4,4'-[(6,11-dioxo-2-(trifluoromethyl)-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-3,8-diyl)bis(azo)]bis[3-hydroxy-N-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



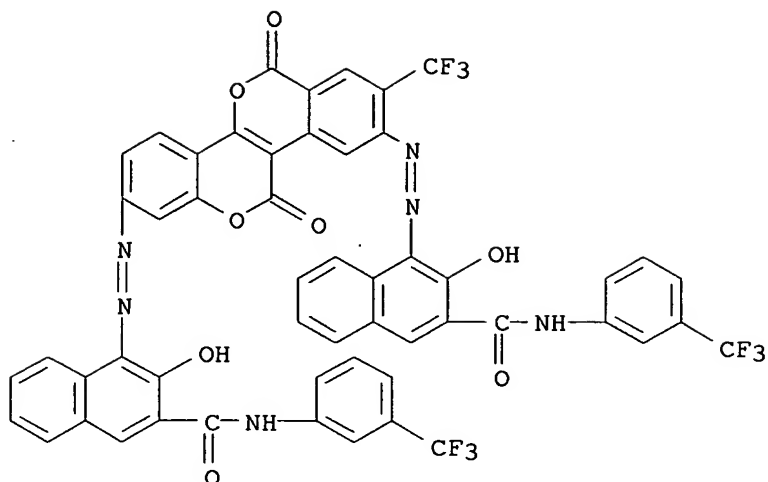
RN 157687-39-3 CAPLUS

CN 2-Naphthalenecarboxamide, 4,4'-[(6,11-dioxo-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-2,9-diyl)bis(azo)]bis[3-hydroxy-N-phenyl- (9CI) (CA INDEX NAME)



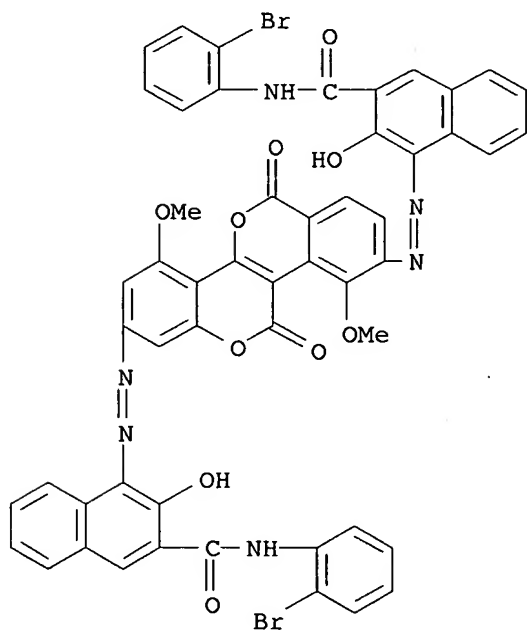
RN 157687-40-6 CAPLUS

CN 2-Naphthalenecarboxamide, 4,4'-[(6,11-dioxo-8-(trifluoromethyl)-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-3,9-diyl)bis(azo)]bis[3-hydroxy-N-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 157687-41-7 CAPLUS

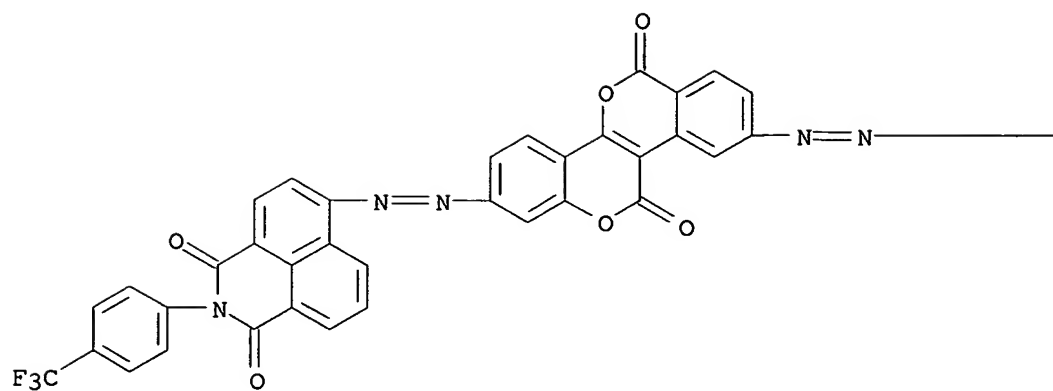
CN 2-Naphthalenecarboxamide, 4,4'-[(4,10-dimethoxy-6,11-dioxo-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-2,9-diyl)bis(azo)]bis[N-(2-bromophenyl)-3-hydroxy- (9CI) (CA INDEX NAME)



RN 157959-55-2 CAPLUS

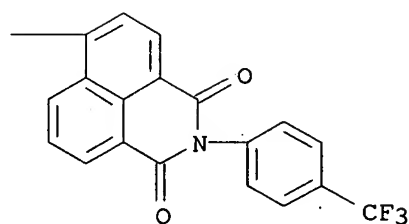
CN 1H-Benz[de]isoquinoline-1,3(2H)-dione, 6,6'-[(6,11-dioxo-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-2,9-diyl)bis(azo)]bis[hydroxy-2-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

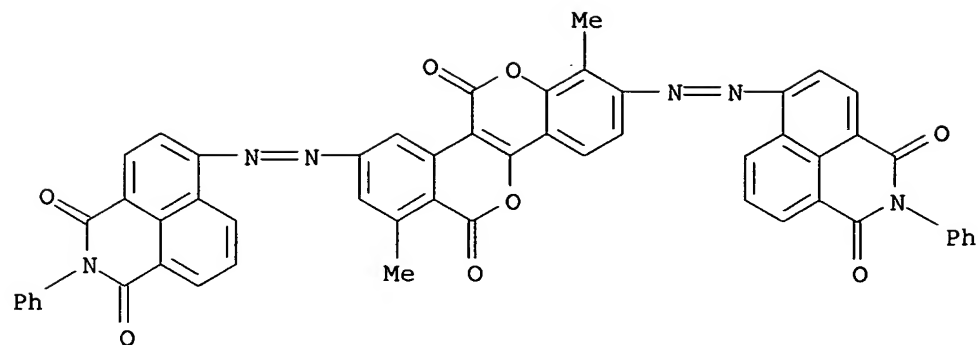


2 ( D1-OH )

PAGE 1-B



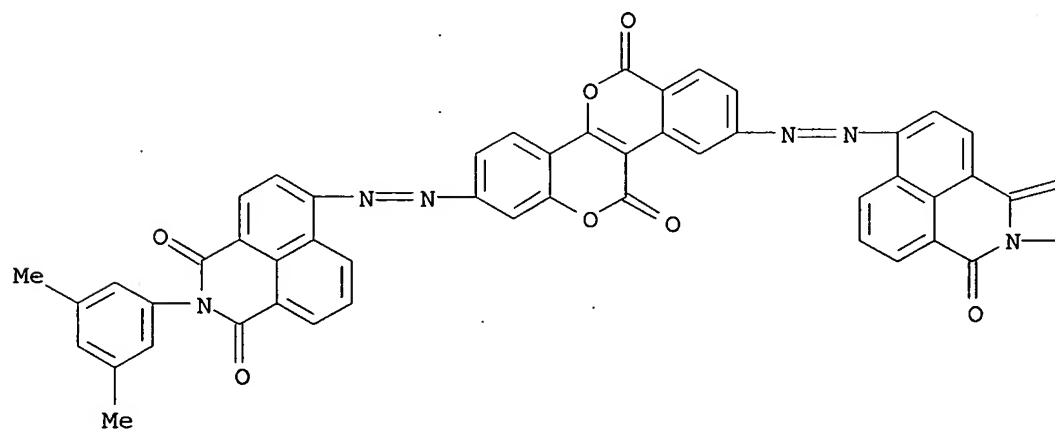
RN 157959-56-3 CAPLUS  
 CN 1H-Benz[de]isoquinoline-1,3(2H)-dione, 6,6'-[(1,7-dimethyl-6,11-dioxo-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-2,9-diyl)bis(azo)]bis[hydroxy-2-phenyl- (9CI) (CA INDEX NAME)



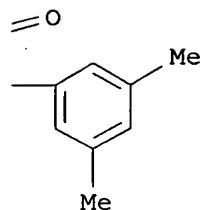
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RN 157959-57-4 CAPLUS  
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PAGE 1-A

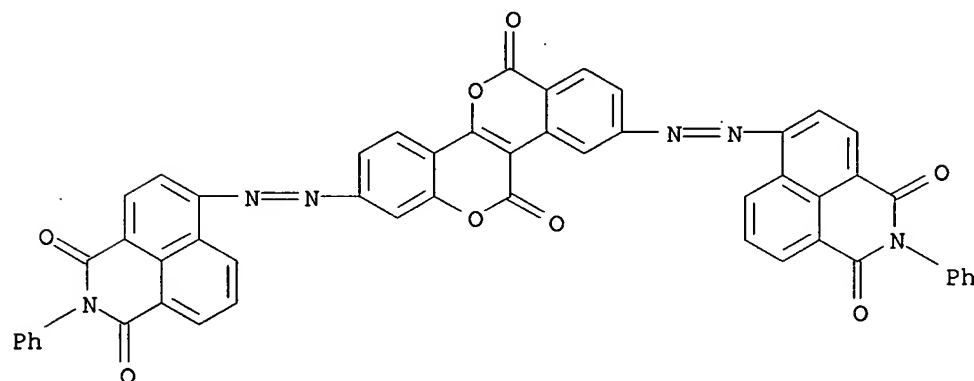


2 ( D1-OH )



RN 157959-58-5 CAPLUS

CN 1H-Benz[de]isoquinoline-1,3(2H)-dione, 6,6'-[(6,11-dioxo-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-2,9-diyl)bis(azo)]bis[hydroxy-2-phenyl-(9CI) (CA INDEX NAME)

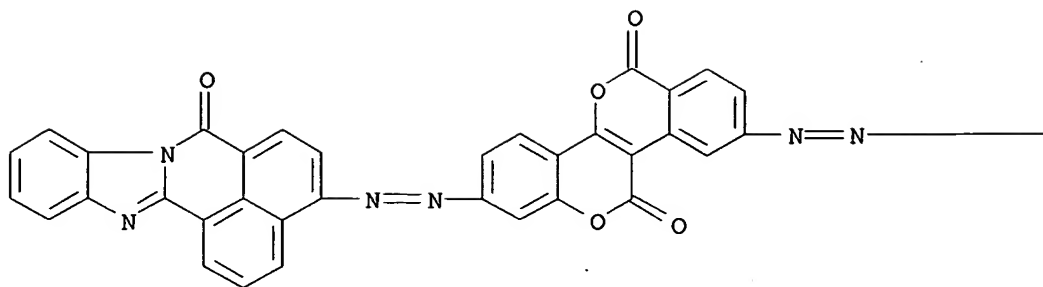


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RN 157959-59-6 CAPLUS

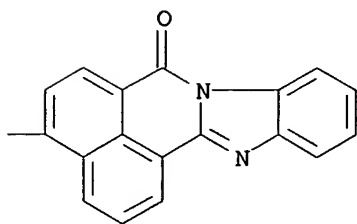
CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 2,9-bis[(hydroxy-7-oxo-7H-benzimidazo[2,1-a]benz[de]isoquinolin-4-yl)azo]- (9CI) (CA INDEX NAME)

PAGE 1-A



2 ( D1-OH )

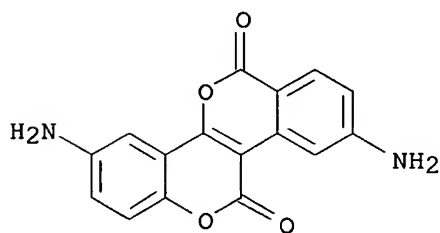
PAGE 1-B



IT 157687-42-8 157687-43-9 157687-44-0

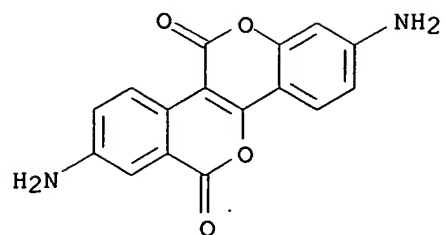
RL: RCT (Reactant); RACT (Reactant or reagent)  
(diazo coupling of, with naphthol derivative)

RN 157687-42-8 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 3,9-diamino- (9CI)  
(CA INDEX NAME)

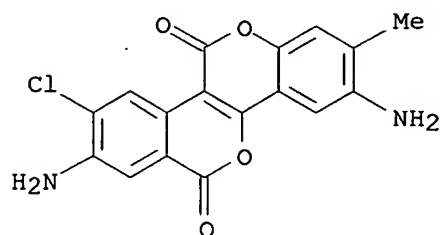
RN 157687-43-9 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 2,8-diamino- (9CI)  
(CA INDEX NAME)



RN 157687-44-0 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 3,8-diamino-9-chloro-2-methyl- (9CI) (CA INDEX NAME)





~~122~~ ANSWER 26 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1991:492008 CAPLUS

DOCUMENT NUMBER: 115:92008

TITLE: Diels-Alder reactions of 2-[(trialkylsilyl)oxy]pyrylium cations of 2H-pyran-2-one and 2H-1-benzopyran-2-one derivatives

AUTHOR(S): Ohkata, Katsuo; Lee, Yong Gyun; Utsumi, Yukinori; Ishimaru, Kenji; Akiba, Kinuya

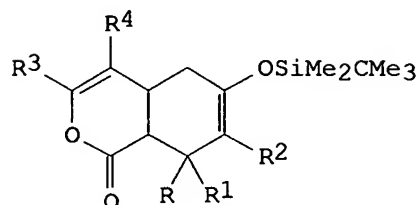
CORPORATE SOURCE: Fac. Sci., Hiroshima Univ., Hiroshima, 730, Japan  
SOURCE: Journal of Organic Chemistry (1991), 56(17), 5052-9  
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 115:92008

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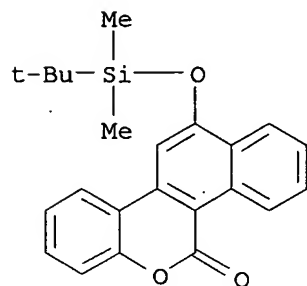
AB The reactions of 6-methyl-2H-pyran-2-one and 2H-1-benzopyran-2-one with  $RR_1C(:CH_2)OSiMe_2CMe_3$  [ $R, R_1 = H, Me, Ph, R_2 = H; R = H, R_1R_2 = (CH_2)_n, n = 3, 4$ ] in the presence of  $Me_3CSiMe_2O_3SCF_3$  gave 30-68% [4 + 2] cycloadducts I [ $R_3 = Me, R_4 = H; R_3R_4 = (CH:CH)_2$ ] regio- and stereoselectively. The ring junction in the cycloadducts is cis. Similar reactions of 3-(ethoxycarbonyl)-2-pyrones and 3-(alkoxycarbonyl)coumarins with the 2-(trialkylsilyl)oxy dienes gave 30-80% cycloadducts.

IT 130043-16-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 130043-16-2 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-5-one, 12-[[[1,1-dimethylethyl)dimethylsilyl]oxy]- (9CI) (CA INDEX NAME)



~~102~~ ANSWER 27 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1990:591715 . CAPLUS

DOCUMENT NUMBER: 113:191715

TITLE: Synthesis of oxasteroidal skeletons by (4+2) type cycloaddition of coumarin and 6-methyl-2-pyrone with siloxydienes mediated by tert-butyldimethylsilyl triflate

AUTHOR(S): Lee, Yong Gyun; Utsumi, Yukinori; Ohkata, Katsuo; Akiba, Kinya

CORPORATE SOURCE: Fac. Sci., Hiroshima Univ., Hiroshima, 730, Japan

SOURCE: Heterocycles (1990), 30(2, Spec. Issue), 813-16

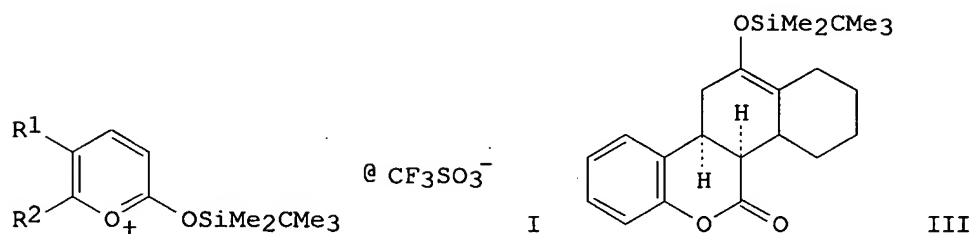
CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:191715

GI



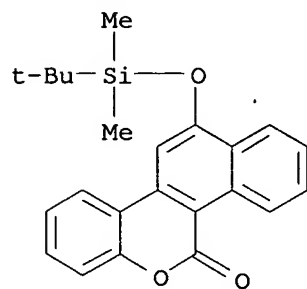
AB A new simple methodol. is described for the preparation of oxasteroidal skeletons containing a lactone ring via cycloaddn. of pyrylium triflates I ( $\text{R}^1\text{R}^2 = \text{CH:CHCH:CH}$ ;  $\text{R}^1 = \text{H}$ ,  $\text{R}^2 = \text{Me}$ ) with siloxydienes  $\text{H}_2\text{C:C(OSiMe}_2\text{CMe}_3)\text{CR}_3\text{:CR}_4\text{R}_5$  [II;  $\text{R}_3 = \text{R}_5 = \text{H}$ ,  $\text{R}_4 = \text{Ph}$ ;  $\text{R}_3 = \text{H}$ ,  $\text{R}_4 = \text{R}_5 = \text{Me}$ ;  $\text{R}_3\text{R}_4 = (\text{CH}_2)_3$ ,  $(\text{CH}_2)_4$ ,  $\text{R}_5 = \text{H}$ ]. Thus, the [4+2] cycloaddn. of I ( $\text{R}^1\text{R}^2 = \text{CH:CHCH:CH}$ ) with II [ $\text{R}_3\text{R}_4 = (\text{CH}_2)_4$ ,  $\text{R}_5 = \text{H}$ ] gave oxasteroid III.

IT 130043-16-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 130043-16-2 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-5-one, 12-[[1,1-dimethylethyl)dimethylsilyl]oxy]- (9CI) (CA INDEX NAME)



10/307,735

~~122~~ ANSWER 28 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1990:55337 CAPLUS

DOCUMENT NUMBER: 112:55337

TITLE: The stereochemistry of pterocarpanoids. A theoretical study

AUTHOR(S): Schoening, Axel; Friedrichsen, Willy

CORPORATE SOURCE: Inst. Org. Chem., Univ. Kiel, Kiel, D-2300, Fed. Rep. Ger.

SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences (1989); 44(8), 975-82  
CODEN: ZNBSEN; ISSN: 0932-0776

DOCUMENT TYPE: Journal

LANGUAGE: German

AB Calcns. (AM 1, mol. mechanics) on pterocarpanoids and related compds. (homo-, hetero-analogs) are reported.

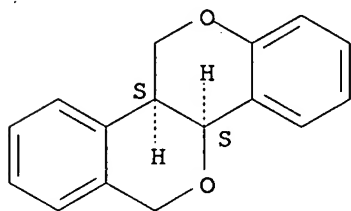
IT 124692-93-9 124692-94-0 124693-01-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
(heat of formation and mol. mechanics calcns. on)

RN 124692-93-9 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran, 4b,10b-dihydro-, cis- (9CI)  
(CA INDEX NAME)

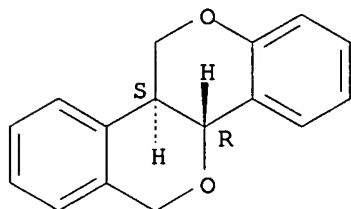
Relative stereochemistry.



RN 124692-94-0 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran, 4b,10b-dihydro-, trans- (9CI)  
(CA INDEX NAME)

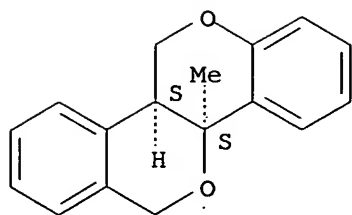
Relative stereochemistry.



RN 124693-01-2 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran, 4b,10b-dihydro-4b-methyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



122 ANSWER 29 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:406441 CAPLUS

DOCUMENT NUMBER: 109:6441

TITLE: New heterocyclic system from salol and phenylacetic acid

AUTHOR(S): Sardesai, Lina G.; Paknikar, Shashikumar K.; Bates, Robert B.; Siahann, Teruna J.; Kane, Vinayak V.; Mishra, Prasana K.

CORPORATE SOURCE: Dep. Chem., Goa Univ., Goa, 403 005, India

SOURCE: Heterocycles (1987), 26(11), 2941-4

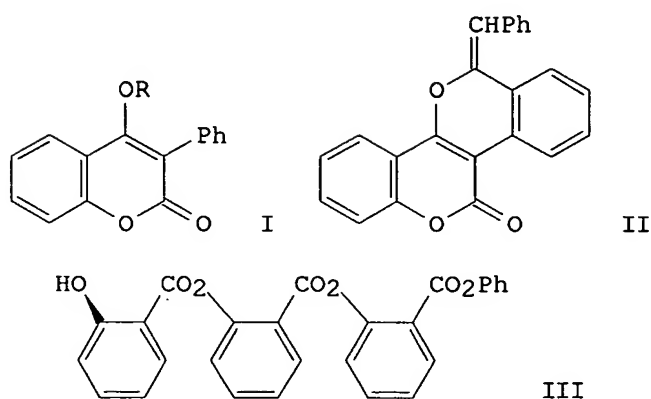
CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:6441

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AB Heating 2-HOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Ph with PhCH<sub>2</sub>CO<sub>2</sub>Ph in Ph<sub>2</sub>O gave 28% 2-(PhCH<sub>2</sub>CO<sub>2</sub>)C<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Ph, 7% 4-hydroxy-3-phenylcoumarin (I, R = H), 10% the benzylidenecoumarinobenzopyranone II, 11% trisalicylide and 6% the oligomeric ester III. Treatment of 2-HOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Ph with PhCH<sub>2</sub>CO<sub>2</sub>H gave a similar spectrum of products along with I (R = PhCH<sub>2</sub>CO), however, yields were less.

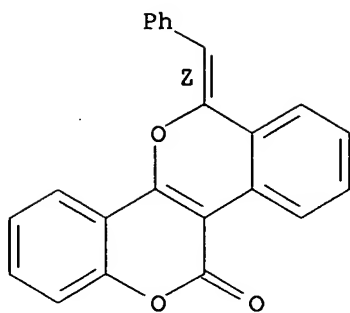
IT 114832-91-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 114832-91-6 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-11-one, 6-(phenylmethylene)-,  
(Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



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L22 ANSWER 30 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1987:176209 CAPLUS

DOCUMENT NUMBER: 106:176209

TITLE: Synthesis of coumarino[4',3':3,4]isocoumarins, coumarino[7',6':3,4]isocoumarins and dibenzo- $\alpha$ -pyrones

AUTHOR(S): Rani, B. S. Uma; Darbarwar, Malleshwar

CORPORATE SOURCE: Dep. Chem., Osmania Univ., Hyderabad, 500 007, India

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1986), 25B(6), 619-22

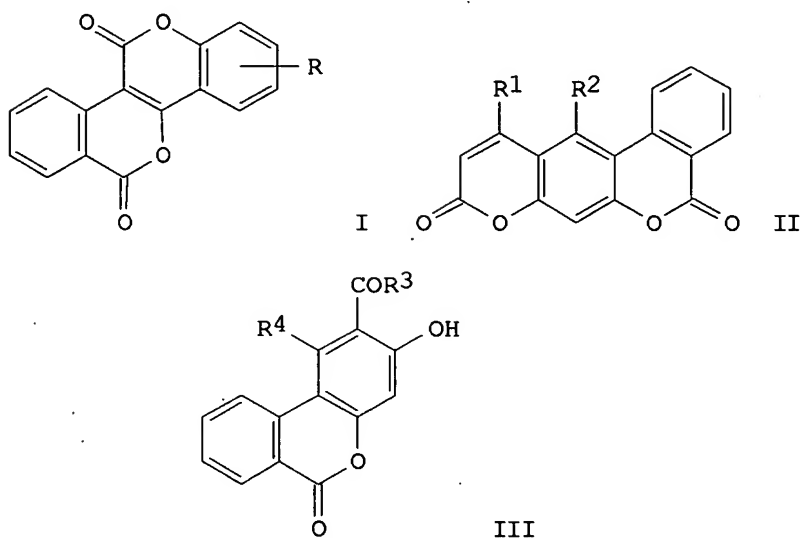
CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 106:176209

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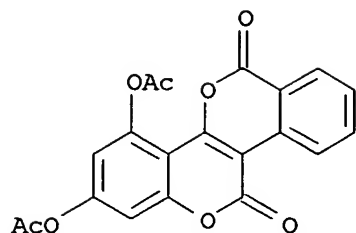
AB Coumarinoisocoumarins I [R = 2-OH, 3-OH, 4-OH, 2,4-(OH)<sub>2</sub>] and II (R<sub>1</sub> = R<sub>2</sub> = H, OH; R<sub>1</sub> = OH, R<sub>2</sub> = H), dibenzo- $\alpha$ -pyrones III (R<sub>3</sub> = H, Me; R = H; R<sub>3</sub> = Me, R<sub>4</sub> = OH) were prepared by the condensation of reactive phenols with 2-bromobenzoic acid in the presence of CuSO<sub>4</sub> as catalyst, and screened for antibacterial and antifungal activity. I [R = 4-OH, 2,4-(OAc)<sub>2</sub>] and II (R<sub>1</sub> = OH, OAc; R<sub>2</sub> = H; R<sub>1</sub> = R<sub>2</sub> = OAc) were most active against Staphylococcus aureus and Escherichia coli; I (R = 2-OAc 3-OAc) and II (R<sub>1</sub> = OAc, R<sub>2</sub> = H; R<sub>1</sub> = R<sub>2</sub> = OAc) were most active against Aspergillus niger at 100 ppm concentration

IT 107125-08-6 107125-10-0 107125-11-1

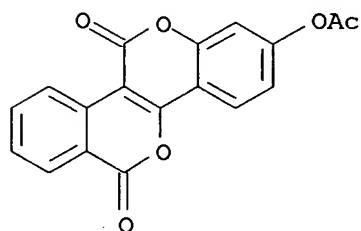
RL: RCT (Reactant); RACT (Reactant or reagent)  
(antibacterial and antifungal activity of)

RN 107125-08-6 CAPLUS

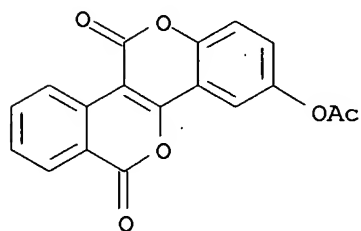
CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 2,4-bis(acetyloxy)-(9CI) (CA INDEX NAME)



RN 107125-10-0 CAPLUS  
 CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 2-(acetyloxy)- (9CI)  
 (CA INDEX NAME)

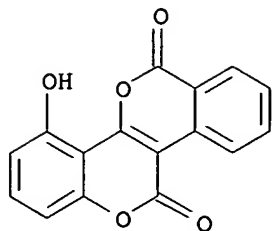


RN 107125-11-1 CAPLUS  
 CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 3-(acetyloxy)- (9CI)  
 (CA INDEX NAME)

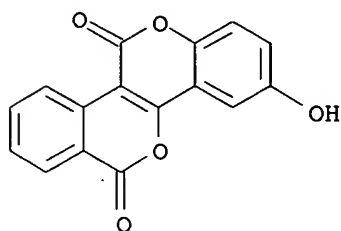


IT 107124-97-0P 107124-98-1P 107124-99-2P  
 107125-00-8P 107125-01-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and antibacterial and antifungal activity of)  
 RN 107124-97-0 CAPLUS  
 CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 4-hydroxy- (9CI)  
 (CA INDEX NAME)

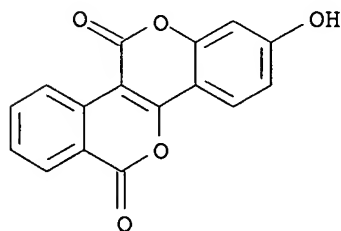




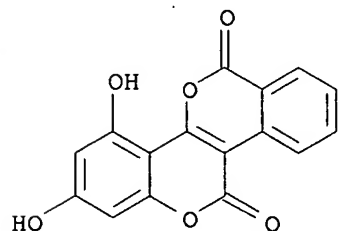
RN 107124-98-1 CAPLUS  
 CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 3-hydroxy- (9CI)  
 (CA INDEX NAME)



RN 107124-99-2 CAPLUS  
 CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 2-hydroxy- (9CI)  
 (CA INDEX NAME)



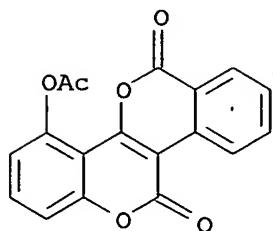
RN 107125-00-8 CAPLUS  
 CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 2,4-dihydroxy- (9CI)  
 (CA INDEX NAME)



RN 107125-01-9 CAPLUS  
 CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 4-(acetyloxy)- (9CI)

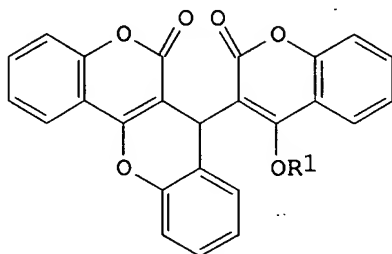
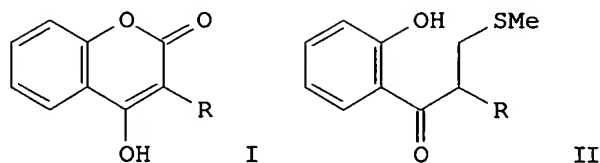
10/307,735

(CA INDEX NAME)



10/307,735

122 ANSWER 31 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1985:220702 CAPLUS  
DOCUMENT NUMBER: 102:220702  
TITLE: Reaction of dimethyl sulfoxide and acetic anhydride  
with 3-substituted 4-hydroxycoumarins  
AUTHOR(S): Khan, Khaliquz Zaman; Tasneem, Khalida; Rahman,  
Mujeebur; Prakash, Satya; Zaman, Asif  
CORPORATE SOURCE: Dep. Res. Unani Med., Aligarh Muslim Univ., Aligarh,  
202 001, India  
SOURCE: Indian Journal of Chemistry, Section B: Organic  
Chemistry Including Medicinal Chemistry (1985),  
24B(1), 42-6  
CODEN: IJSBDB; ISSN: 0376-4699  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 102:220702  
GI



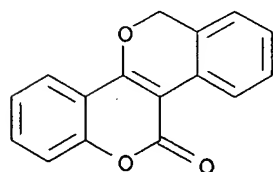
AB 4-Hydroxycoumarins I (R = Ph, allyl), treated with Me<sub>2</sub>SO-Ac<sub>2</sub>O, gave 2-hydroxyphenyl-1-methylthioprop-3-ones II. The same reagent, modified by prior heating, reacted with 6H,7H-7-(4-hydroxy-3-coumaranyl)[1]benzopyrano[4,3-b][1]benzopyranone III (R<sub>1</sub> = H) to give fragmentation products. Reagent unmodified by heating gave only O-acylation product III (R<sub>1</sub> = Ac) with no fragmentation.

IT 96600-94-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 96600-94-1 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-11-one (9CI) (CA INDEX NAME)



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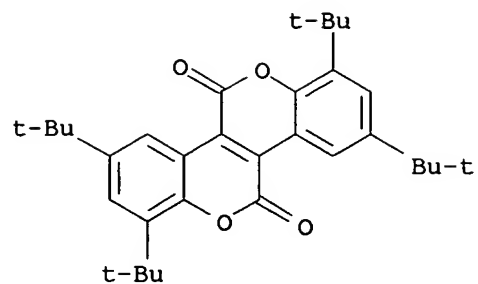
~~L22~~



IT

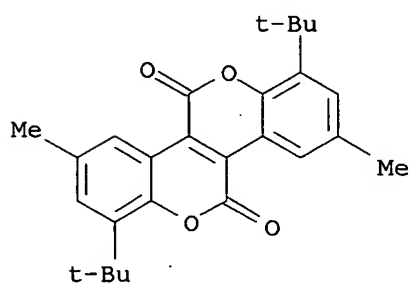


CN



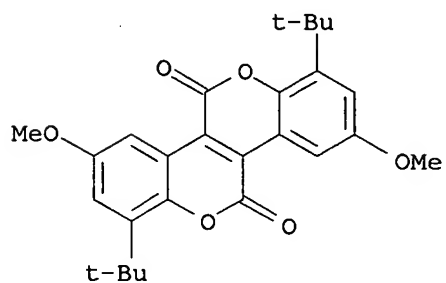
RN 80360-51-6 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 1,7-bis(1,1-dimethylethyl)-3,9-dimethyl- (9CI) (CA INDEX NAME)



RN 80360-52-7 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 1,7-bis(1,1-dimethylethyl)-3,9-dimethoxy- (9CI) (CA INDEX NAME)



L72 ANSWER 33 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1984:120827 CAPLUS

DOCUMENT NUMBER: 100:120827

TITLE: A synthesis of bikaverin (7,12-dihydro-6,11-dihydroxy-3,8-dimethoxy-1-methyl-10H-benzo[b]xanthene-7,10,12-trione) and some related benzoxanthenes and quinones

AUTHOR(S): Kjaer, Dana; Kjaer, Anders; Risbjerg, Elizabeth

CORPORATE SOURCE: Dep. Org. Chem., Tech. Univ. Denmark, Lyngby, 2800, Den.

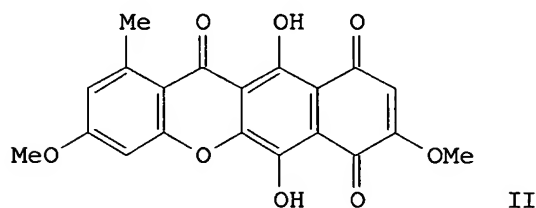
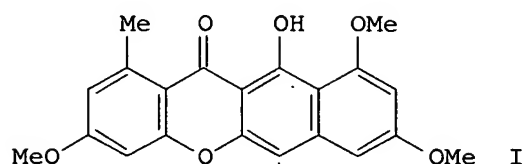
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1983), (11), 2815-20

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



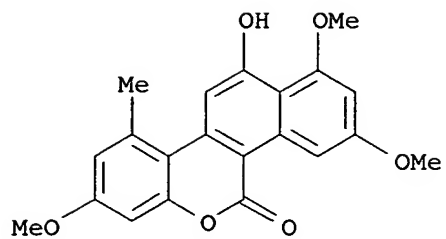
AB Cyclocondensation reaction of 2-hydroxy-4-methoxy-6-methylacetophenone with di-Me 3,5-dimethoxyhomophthalate and NaH in refluxing THF for 15 h gave 20-25% benzoxanthone I, which on oxidation with F3CC(O)OOH in CHCl3 at 0° for 6 h gave 38% bikaverin (II), a biol. interesting fungal pigment, and 37% of its 16-deoxy derivative. Five other 11-hydroxybenzoxanthenes were prepared by similar cyclocondensation of hydroxyacetophenones and di-Me homophthalates; 4 of these were oxidized to the corresponding quinones.

IT 89141-05-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 89141-05-9 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]pyran-5-one, 12-hydroxy-1,3,8-trimethoxy-10-methyl- (9CI) (CA INDEX NAME)



10/307,735

~~122~~ ANSWER 34 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1982:162487 CAPLUS

DOCUMENT NUMBER: 96:162487

TITLE: Pechmann reaction of 4-hydroxycoumarins and thiocoumarins with cyclohexanone and ethyl cyclopentanone-2-carboxylates

AUTHOR(S): Merchant, J. R.; Koshti, N. M.; Bakre, K. M.

CORPORATE SOURCE: Dep. Chem., Inst. Sci., Bombay, 400032, India

SOURCE: Journal of Heterocyclic Chemistry (1981), 18(8), 1655-8

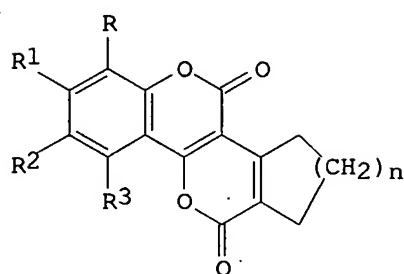
CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

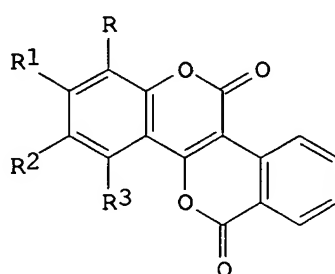
LANGUAGE: English

OTHER SOURCE(S): CASREACT 96:162487

GI



I



II

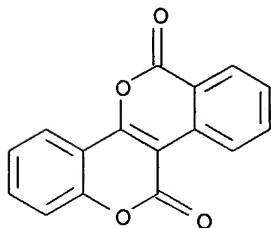
AB The Pechmann reaction of 4-hydroxycoumarins with Et cyclohexanone-2-carboxylate and Et cyclopentanone-2-carboxylate gave benzopyranopyrandonones I (R, R1, R2, R3 = H, Me; n = 2, 1; resp.). Dehydrogenation of I (n = 2) gave benzopyranobenzopyrandonones II. Anticoagulant activity of I was poor.

IT 2288-98-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and hydrolysis of)

RN 2288-98-4 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione (8CI, 9CI) (CA INDEX NAME)



IT 27284-76-0P 27284-78-2P 27284-80-6P

81450-24-0P

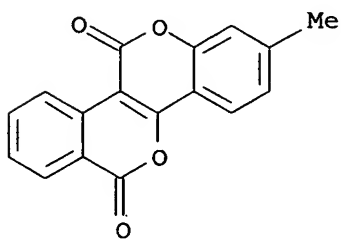
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)



10/307,735

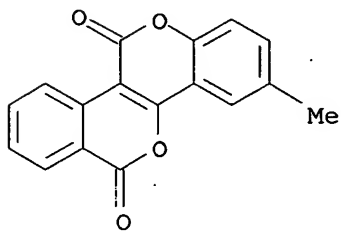
RN 27284-76-0 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 2-methyl- (8CI, 9CI)  
(CA INDEX NAME)



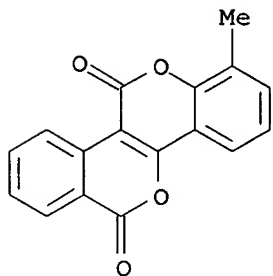
RN 27284-78-2 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 3-methyl- (8CI, 9CI)  
(CA INDEX NAME)



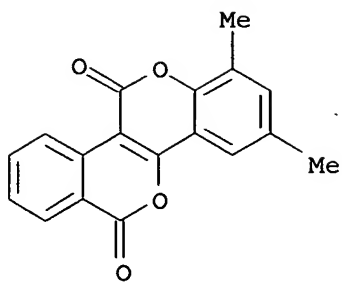
RN 27284-80-6 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 1-methyl- (8CI, 9CI)  
(CA INDEX NAME)



RN 81450-24-0 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 1,3-dimethyl- (9CI)  
(CA INDEX NAME)



L29 ANSWER 35 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1982:104011 CAPLUS

DOCUMENT NUMBER: 96:104011

TITLE: Oxidative conversions of 2,2'-diphenoquinone valence isomers with 2,3-dichloro-5,6-dicyanobenzoquinone. Synthesis and spectroscopic properties of (E)-(3,3')dibenzofuranylidene-2,2'-diones (isoxindigos)

AUTHOR(S): Becker, Hans Dieter; Lingnert, Hans

CORPORATE SOURCE: Dep. Org. Chem., Chalmers Univ. Technol., Gothenburg, S-412 96, Swed.

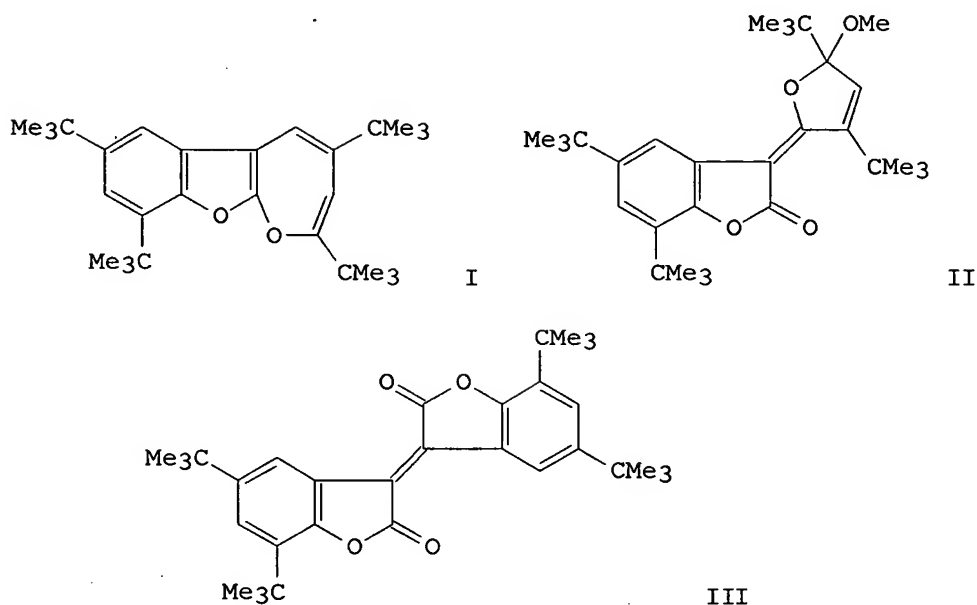
SOURCE: Journal of Organic Chemistry (1982), 47(6), 1095-101  
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 96:104011

GI



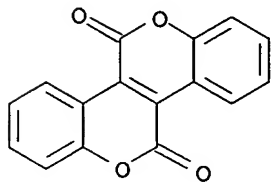
AB Oxepinobenzofurans (e.g. I), derived from tetraalkyl-substituted and dialkyldimethoxy-substituted 2,2'-diphenoquinones by spontaneous valence isomerization, react with 2,3-dichloro-5,6-dicyanobenzoquinone (DDQ) in the presence of water to give benzofuranylidene-2-ones (e.g. II) whose formation involves hydrolysis of the substrate ketal moiety. The course of the reaction and, consequently, the structure of the oxidation products depend on the nature of the substrate substituents. Upon exhaustive oxidation by DDQ, benzofuranylidene-2-ones are smoothly converted into isoxindigos (e.g. III). A mechanism for their formation involving hydration of the exocyclic double bond, oxidative coupling, and loss of the side chain by a retro-aldol reaction is proposed. The electron spectral properties of isoxindigos and those of their isomeric dibenzonaphthyrone are compared and discussed.

IT 13225-81-5P 80360-50-5P 80360-51-6P  
80360-52-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and reduction of)

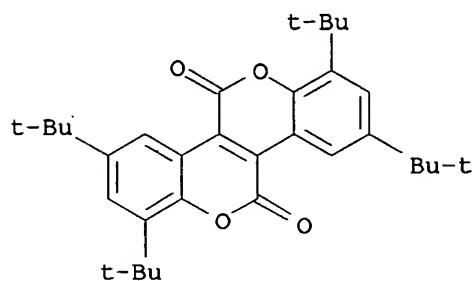
RN 13225-81-5 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione (8CI, 9CI) (CA INDEX NAME)



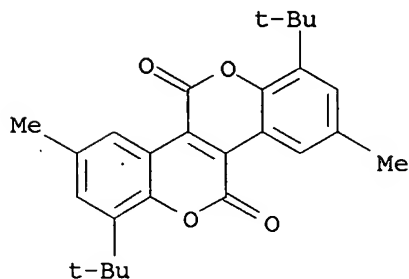
RN 80360-50-5 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 1,3,7,9-tetrakis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



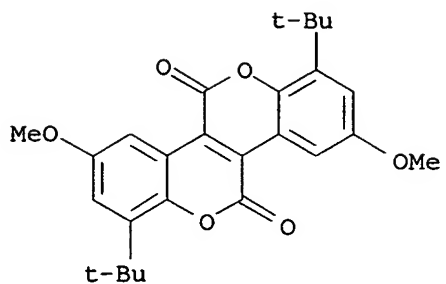
RN 80360-51-6 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 1,7-bis(1,1-dimethylethyl)-3,9-dimethyl- (9CI) (CA INDEX NAME)



RN 80360-52-7 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 1,7-bis(1,1-dimethylethyl)-3,9-dimethoxy- (9CI) (CA INDEX NAME)



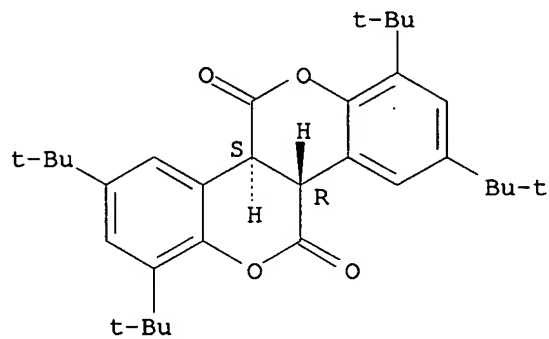
IT **80360-55-0P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 80360-55-0 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 1,3,7,9-tetrakis(1,1-dimethylethyl)-4b,10b-dihydro-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



10/307,735

~~L2~~ ANSWER 36 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1981:30595 CAPLUS

DOCUMENT NUMBER: 94:30595

TITLE: Synthesis of isocoumarines from phenylmalonyl heterocyclics

AUTHOR(S): Stadlbauer, Wolfgang; Ghobrial, Nadia; Kappe, Thomas

CORPORATE SOURCE: Inst. Org. Chem., Univ. Graz, Graz, A-8010, Austria

SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie (1980), 35B(7), 892-5  
CODEN: ZNBAD2; ISSN: 0340-5087

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 94:30595

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

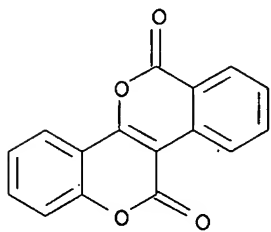
AB Heating quinolones I (R = H, Me, Ph) with CO(OPh)<sub>2</sub> in 10% Na<sub>2</sub>CO<sub>3</sub> at 300° gave 6H-[2]benzopyrano[4,3-c]quinolines II in 71-82% yields. Similarly benzoquinolizinone III gave IV in 74% yield, phenalenones V (R<sub>1</sub> = R<sub>2</sub> = H; R<sub>1</sub> = Ph, R<sub>2</sub> = OH) gave 13-15% VI, and 2-phenyl-3-quinolinol gave 18% VII. Pyridones VIII (R<sub>3</sub> = R<sub>4</sub> = H, R<sub>5</sub> = Me, R<sub>6</sub> = CO<sub>2</sub>Et; R<sub>3</sub> = R<sub>6</sub> = H, R<sub>4</sub> = R<sub>5</sub> = Ph) gave VIII (R<sub>3</sub> = R<sub>4</sub> = Ph, R<sub>5</sub> = Me, R<sub>6</sub> = CO<sub>2</sub>Et; R<sub>3</sub> = R<sub>4</sub> = R<sub>5</sub> = Ph, R<sub>6</sub> = H) in 6% and 25% yields, resp. Heating quinolinone IX (R<sub>3</sub> = H) with NaOAc or 4-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H gave 34% IX (R<sub>3</sub> = Ph) and 6% IX (R<sub>3</sub> = CO<sub>2</sub>Ph).

IT 2288-98-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 2288-98-4 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione (8CI, 9CI) (CA INDEX NAME)



L22 ANSWER 37 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1980:514350 CAPLUS

DOCUMENT NUMBER: 93:114350

TITLE: Quinones and quinone methides. VI. Reactions of 2-(arylmethyl)- and 2-(1-arylethyl)-1,4-benzoquinones with 4-hydroxy-2H-1-benzopyran-2-one

AUTHOR(S): Jurd, Leonard; Wong, Rosalind Y.

CORPORATE SOURCE: Sci. Educ. Adm., West. Reg. Res. Cent., Berkeley, CA, 94710, USA

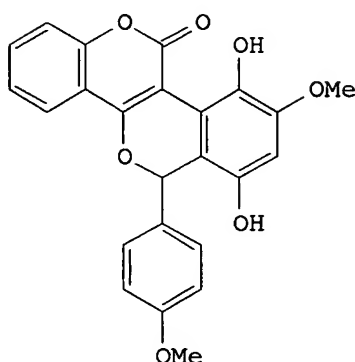
SOURCE: Australian Journal of Chemistry (1980), 33(1), 137-54  
CODEN: AJCHAS; ISSN: 0004-9425

DOCUMENT TYPE: Journal

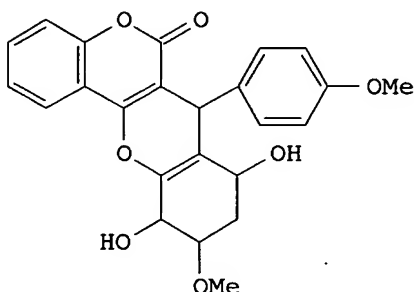
LANGUAGE: English

OTHER SOURCE(S): CASREACT 93:114350

GI



III



IV

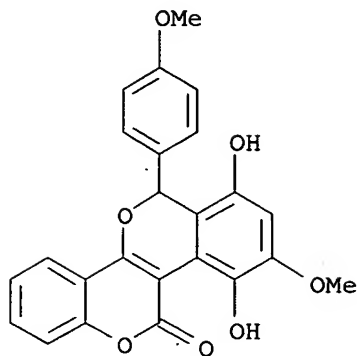
AB In alc. KOH 2-methoxy-5-[(4-methoxyphenyl)methyl]-1,4-benzoquinone (I) reacted with 4-hydroxy-2H-1-benzopyran-2-one (II) to yield the quinol (III). In pyridine, however, I tautomerized the o-quinone methide which combined with II to yield IV. 2-(1-Arylethyl)-1,4-benzoquinones yielded quinols related to III in both alc. KOH and pyridine solns.; this indicates that quinone methides which might be formed from these quinones are relatively unreactive to nucleophiles.

IT 74700-63-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of)

RN 74700-63-3 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 7,10-dihydroxy-8-methoxy-11-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

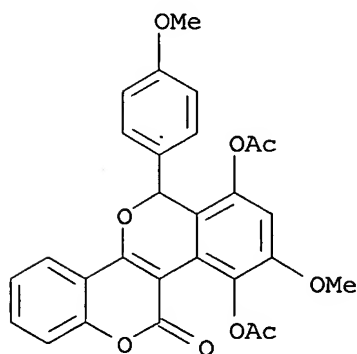


IT 74700-64-4P 74700-65-5P 74700-66-6P  
 74700-68-8P 74700-69-9P 74700-70-2P  
 74700-71-3P 74700-72-4P 74700-74-6P  
 74700-75-7P 74700-76-8P 74700-78-0P  
 74700-79-1P 74701-00-1P 74726-30-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 74700-64-4 CAPLUS

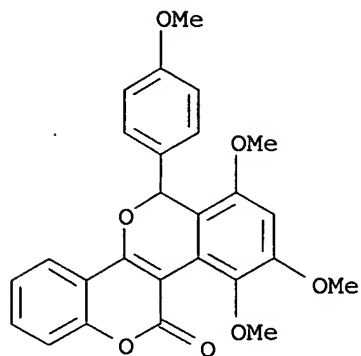
CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 7,11-bis(acetyloxy)-8-methoxy-11-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 74700-65-5 CAPLUS

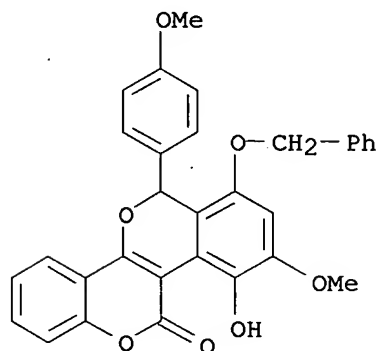
CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 7,8,10-trimethoxy-11-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)





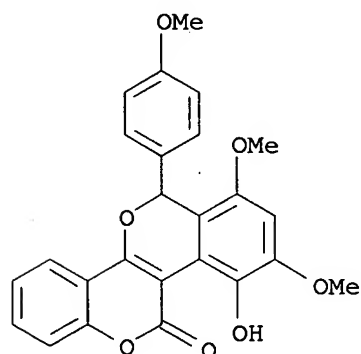
RN 74700-66-6 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 7-hydroxy-8-methoxy-11-(4-methoxyphenyl)-10-(phenylmethoxy)- (9CI) (CA INDEX NAME)



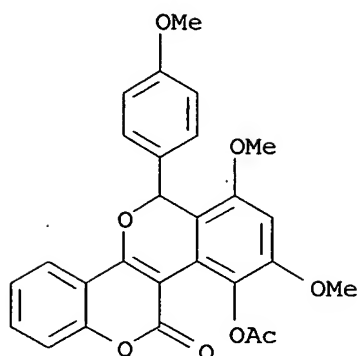
RN 74700-68-8 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 7-hydroxy-8,10-dimethoxy-11-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

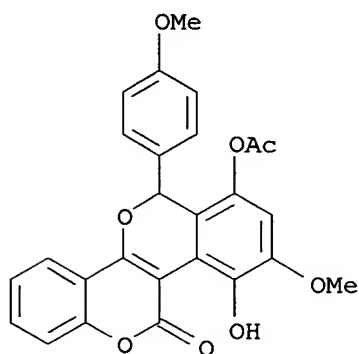


RN 74700-69-9 CAPLUS

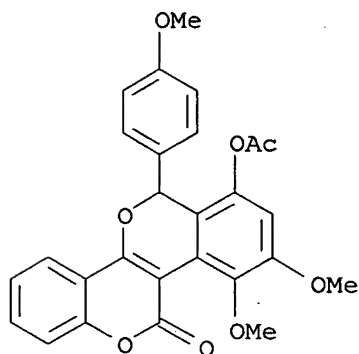
CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 7-(acetyloxy)-8,10-dimethoxy-11-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



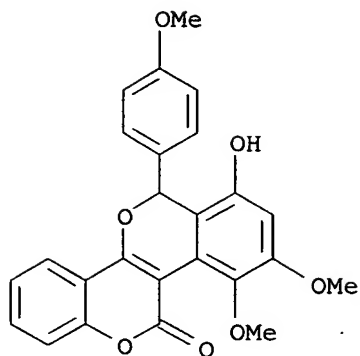
RN 74700-70-2 CAPLUS  
 CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 10-(acetyloxy)-7-hydroxy-8-methoxy-11-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 74700-71-3 CAPLUS  
 CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 10-(acetyloxy)-7,8-dimethoxy-11-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

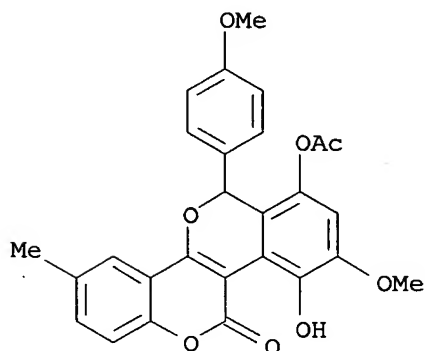


RN 74700-72-4 CAPLUS  
 CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 10-hydroxy-7,8-dimethoxy-11-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



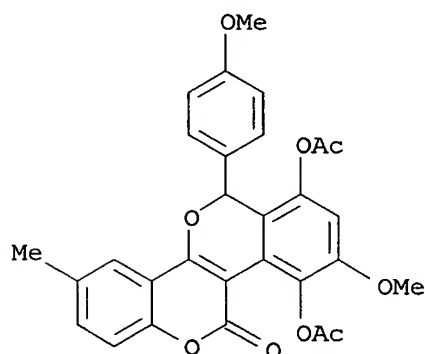
RN 74700-74-6 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 10-(acetyloxy)-7-hydroxy-8-methoxy-11-(4-methoxyphenyl)-2-methyl- (9CI) (CA INDEX NAME)



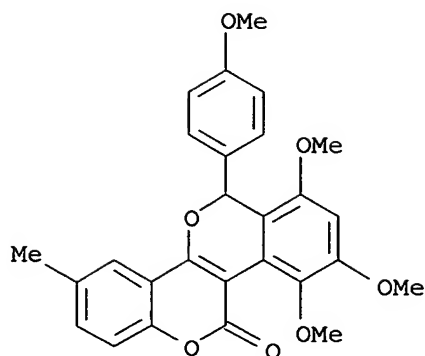
RN 74700-75-7 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 7,10-bis(acetyloxy)-8-methoxy-11-(4-methoxyphenyl)-2-methyl- (9CI) (CA INDEX NAME)



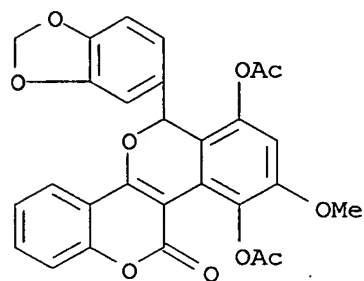
RN 74700-76-8 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 7,8,10-trimethoxy-11-(4-methoxyphenyl)-2-methyl- (9CI) (CA INDEX NAME)



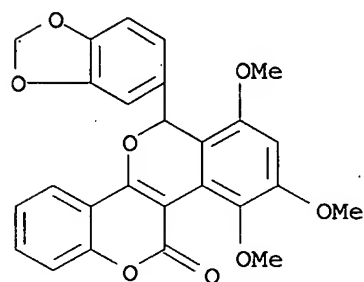
RN 74700-78-0 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 7,10-bis(acetyloxy)-11-(1,3-benzodioxol-5-yl)-8-methoxy- (9CI) (CA INDEX NAME)



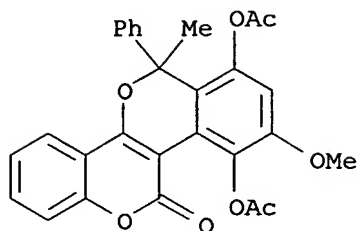
RN 74700-79-1 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 11-(1,3-benzodioxol-5-yl)-7,8,10-trimethoxy- (9CI) (CA INDEX NAME)



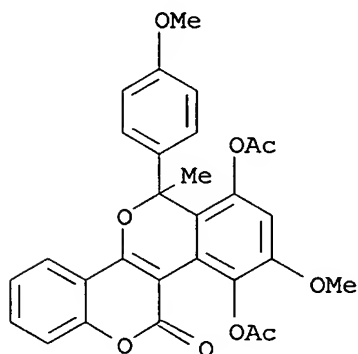
RN 74701-00-1 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 7,10-bis(acetyloxy)-8-methoxy-11-methyl-11-phenyl- (9CI) (CA INDEX NAME)



RN 74726-30-0 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-11-one, 7,10-bis(acetyloxy)-9-methoxy-6-(4-methoxyphenyl)-6-methyl- (9CI) (CA INDEX NAME)

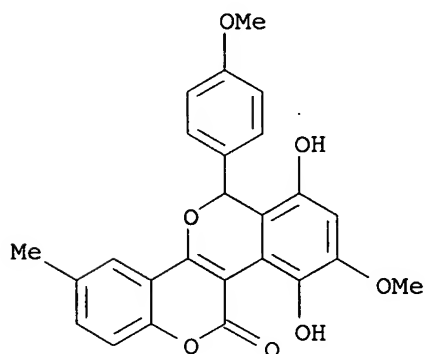


IT 74700-73-5P 74700-77-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation, acetylation and methylation of)

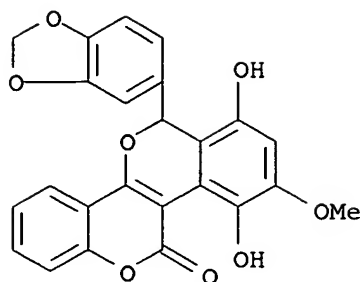
RN 74700-73-5 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 7,10-dihydroxy-8-methoxy-11-(4-methoxyphenyl)-2-methyl- (9CI) (CA INDEX NAME)



RN 74700-77-9 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 11-(1,3-benzodioxol-5-yl)-7,10-dihydroxy-8-methoxy- (9CI) (CA INDEX NAME)

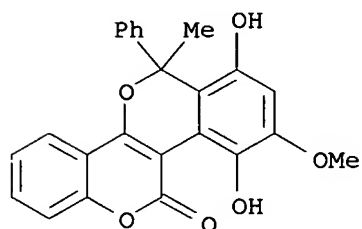


IT 74700-99-5P 74701-04-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation, acetylation and oxidation of)

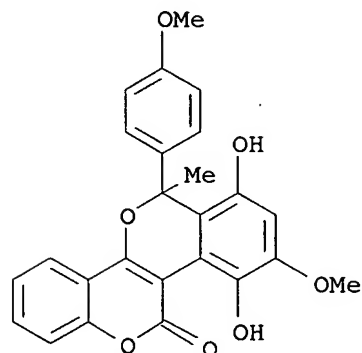
RN 74700-99-5 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 7,10-dihydroxy-8-methoxy-11-methyl-11-phenyl- (9CI) (CA INDEX NAME)



RN 74701-04-5 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6-one, 7,10-dihydroxy-8-methoxy-11-(4-methoxyphenyl)-11-methyl- (9CI) (CA INDEX NAME)



~~L22~~ ANSWER 38 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1980:76356 CAPLUS

DOCUMENT NUMBER: 92:76356

TITLE: Photooxygenation of flavanonol-red related compounds

AUTHOR(S): Shibata, Kozo; Ichikawa, Nobutaka; Kubota, Takashi

CORPORATE SOURCE: Fac. Sci., Osaka City Univ., Osaka, 558, Japan

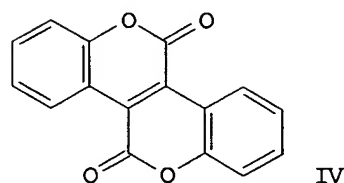
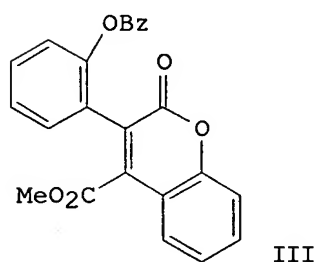
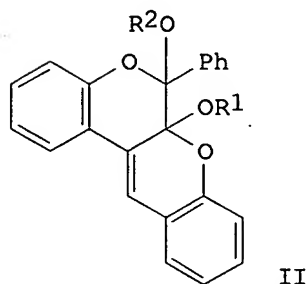
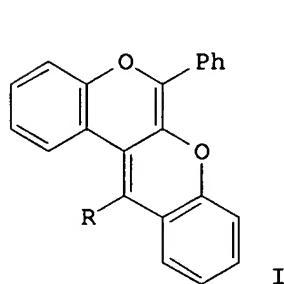
SOURCE: Chemistry Letters (1979), (10), 1301-4

CODEN: CMLTAG; ISSN: 0366-7022

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



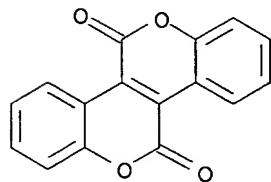
AB Photolysis of the dioxabenzanthracene I (R = H) in EtOH in air gave II (R1 = R2 = Et) which underwent methanolysis to II (R1 = R2 = Me). Photooxidn. of I (R = H) in EtOH followed by recrystn. from MeOH gave II (R1 = Me, R2 = Et). I (R = CO2Me) was not photolyzed under the above conditions, but in the presence of Rose Bengal it gave the lactone III, which on alkaline hydrolysis gave the dilactone IV.

IT 13225-81-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 13225-81-5 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione (8CI, 9CI) (CA INDEX NAME)



10/307,735

~~10~~2 ANSWER 39 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1979:474500 CAPLUS

DOCUMENT NUMBER: 91:74500

TITLE: Photooxygenation of flavanonol-red and unusual autoxidation of photoflavanonol-red

AUTHOR(S): Shibata, Kozo; Matsuo, Kotaro; Ichikawa, Nobutaka; Kubota, Takashi

CORPORATE SOURCE: Fac. Sci., Osaka City Univ., Osaka, 558, Japan

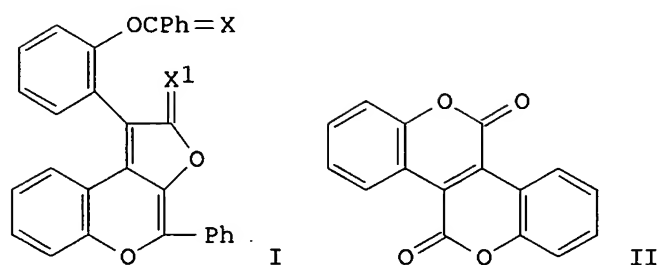
SOURCE: Chemistry Letters (1979), (5), 511-14

CODEN: CMLTAG; ISSN: 0366-7022

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



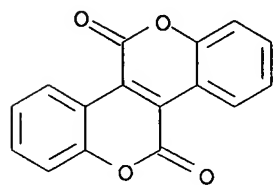
AB Photooxidn. of flavanonol red (I, XX1 = bond) occurred with singlet O to give photoflavanonol red (I, X = X1 = O). The latter compound autoxidized in alkaline solution to the dibenzonaphthyrone II.

IT 13225-81-5P

RL: FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, by autoxidn. of photoflavanonol red)

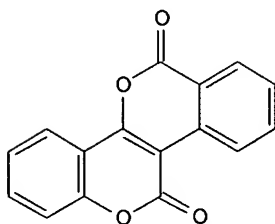
RN 13225-81-5 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione (8CI, 9CI) (CA INDEX NAME)



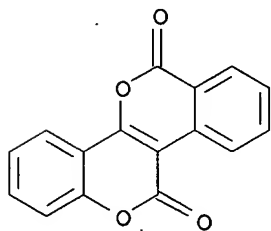


~~LE2~~ ANSWER 40 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1979:103871 CAPLUS  
 DOCUMENT NUMBER: 90:103871  
 TITLE: A by-product in the synthesis of 4-hydroxy-3-phenylcoumarin  
 AUTHOR(S): Stadlbauer, Wolfgang; Kappe, Thomas  
 CORPORATE SOURCE: Inst. Org. Chem., Univ. Graz, Graz, Austria  
 SOURCE: Monatshefte fuer Chemie (1978), 109(6), 1485-7  
 CODEN: MOCMB7; ISSN: 0026-9247  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 GI

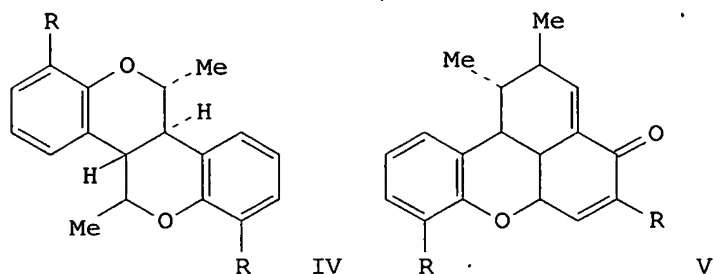


I

AB The synthesis of 4-hydroxy-3-phenylcoumarin (I) from PhOH and PhCH(CO<sub>2</sub>Et)<sub>2</sub> yields the isocoumarin derivative II as a by-product (1-2%). If I is heated with PhCH(CO<sub>2</sub>Et)<sub>2</sub> or di-Ph carbonate at 300° the coumarinoisocoumarin II is formed in 83% and 85% yield, resp.  
 IT **2288-98-4P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 2288-98-4 CAPLUS  
 CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione (8CI, 9CI) (CA INDEX NAME)



~~122~~ ANSWER 41 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1978:120926 CAPLUS  
 DOCUMENT NUMBER: 88:120926  
 TITLE: Oxygen heterocycles by oxidation of ortho-alkylphenols. Oxidation of ortho-propenylphenols  
 AUTHOR(S): Cornia, Mara; Merlini, Lucio; Zanarotti, Antonio  
 CORPORATE SOURCE: Ist. Chim., Politec. Milano, Milan, Italy  
 SOURCE: Gazzetta Chimica Italiana (1977), 107(5-6), 299-304  
 CODEN: GCITA9; ISSN: 0016-5603  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 88:120926  
 GI



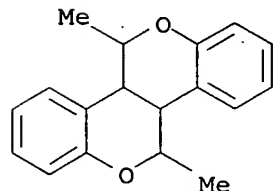
AB Oxidation of 2-propenylphenols by DDQ (I), Ag<sub>2</sub>O (II), or PdCl<sub>2</sub> (III) was studied. I acts as a 2-electron oxidant to form chromenes or spirodibenzopyrans. Use of II gave benzopyranobenzopyrans, e.g., IV (R = Me, H), benzoxanthenones V, and dihydrobenzopyrans via radical phenol coupling. III was inactive except with 2-MeCH:CPhC<sub>6</sub>H<sub>4</sub>OH which gave 2-methyl-3-phenylbenzopyran.

IT 65769-00-8P 65769-04-2P 65769-06-4P  
 65769-07-5P 65831-96-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

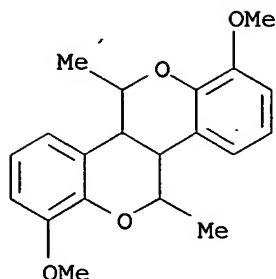
RN 65769-00-8 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran, 4b,5,10b,11-tetrahydro-5,11-dimethyl-, (4b $\alpha$ ,5 $\alpha$ ,10b $\beta$ ,11 $\beta$ )- (9CI) (CA INDEX NAME)



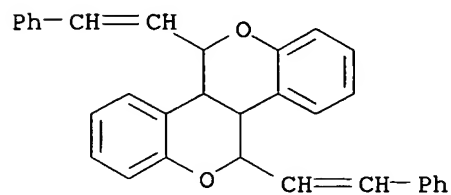
RN 65769-04-2 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran, 4b,5,10b,11-tetrahydro-1,7-dimethoxy-5,11-dimethyl-, (4b $\alpha$ ,5 $\alpha$ ,10b $\beta$ ,11 $\beta$ )- (9CI) (CA INDEX NAME)



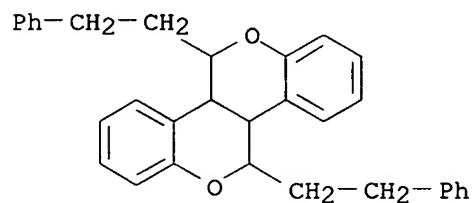
RN 65769-06-4 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran, 4b,5,10b,11-tetrahydro-5,11-bis(2-phenylethenyl)-, [4b $\alpha$ ,5 $\alpha$ (E),10b $\beta$ ,11 $\beta$ (E)]- (9CI) (CA INDEX NAME)



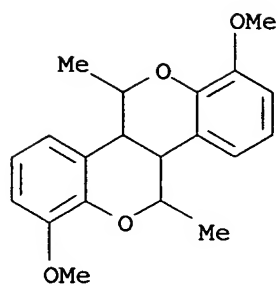
RN 65769-07-5 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran, 4b,5,10b,11-tetrahydro-5,11-bis(2-phenylethyl)-, (4b $\alpha$ ,5 $\alpha$ ,10b $\beta$ ,11 $\beta$ )- (9CI) (CA INDEX NAME)



RN 65831-96-1 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran, 4b,5,10b,11-tetrahydro-1,7-dimethoxy-5,11-dimethyl-, (4b $\alpha$ ,5 $\alpha$ ,10b $\alpha$ ,11 $\alpha$ )- (9CI) (CA INDEX NAME)



122 ANSWER 42 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1976:421173 CAPLUS

DOCUMENT NUMBER: 85:21173

TITLE: Synthesis of oxygen heterocycles by oxidation of ortho-alkylphenols: 2-arylbenzofurans, 4b,9b-dihydrobenzofuro[3,2-b]benzofuran and 4b,5,10b,11-tetrahydropyrano[4,3-c]benzopyrans from hydroxystilbenes

AUTHOR(S): Cardillo, Barbara; Cornia, Mara; Merlini, Lucio

CORPORATE SOURCE: Ist. Chim., Politec. Milano, Milan, Italy

SOURCE: Gazzetta Chimica Italiana (1975), 105(11-12), 1151-63

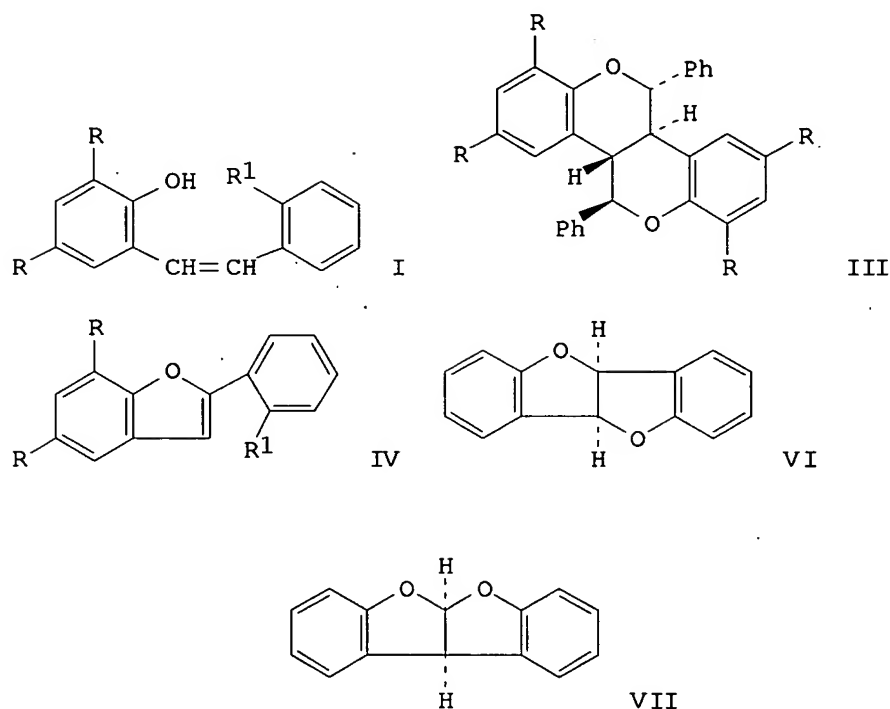
CODEN: GCITA9; ISSN: 0016-5603

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 85:21173

GI



AB Oxidation of hydroxystilbenes I (R = H, Me; R1 = H) with Ag<sub>2</sub>O or 2,3-dichloro-5,6-dicyanobenzoquinone (II) gave benzopyranobenzopyrans III (R = H, Me), but PdCl<sub>2</sub> in aqueous MeOH and AcONa gave benzofuran IV (R = Me, R1 = H). These reactions with I (R = H, R1 = OH) gave mixts. of benzofuran IV (R = H, R1 = OH) (V) and benzofurobenzofuran VI, but treatment of (2-HOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>)<sub>2</sub> gave a mixture of V and its 2,3-dihydro derivative 2-HOC<sub>6</sub>H<sub>4</sub>CHO was reduced with Zn-AcOH to give benzofurobenzofuran VII and V.

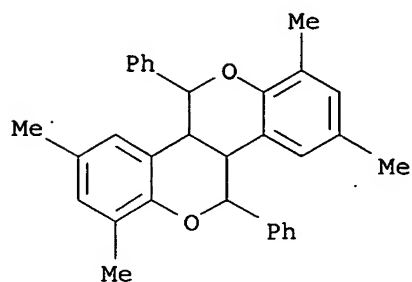
IT 54497-37-9P 59483-18-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 54497-37-9 CAPLUS

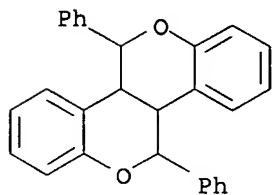
10/307,735

CN [1]Benzopyrano[4,3-c][1]benzopyran, 4b,5,10b,11-tetrahydro-1,3,7,9-tetramethyl-5,11-diphenyl-, (4b $\alpha$ ,5 $\alpha$ ,10b $\beta$ ,11 $\beta$ )- (9CI)  
(CA INDEX NAME)



RN 59483-18-0 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran, 4b,5,10b,11-tetrahydro-5,11-diphenyl- (9CI) (CA INDEX NAME)



L2X ANSWER 43 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1975:50153 CAPLUS

DOCUMENT NUMBER: 82:50153

TITLE: 1,3,7,9-tetramethyl-5,11-diphenyl[1]benzopyrano[4,3-c][1]benzopyran, C32H30O2

AUTHOR(S): Andreetti, G. D.; Bocelli, G.; Coghi, L.; Sgarakotto, P.

CORPORATE SOURCE: Ist. Strutturistica Chim., Univ. Parma, Parma, Italy

SOURCE: Crystal Structure Communications (1974), 3(4), 761-4  
CODEN: CSCMCS; ISSN: 0302-1742

DOCUMENT TYPE: Journal

LANGUAGE: English

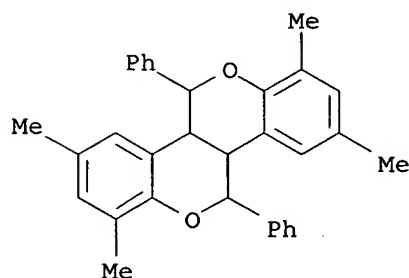
AB Crystals of the title compound have space group P21/c, with  $a$  13.54(1),  $b$  5.270(5),  $c$  21.29(2) Å,  $\beta$  128.7(2)°, and  $Z = 2$ . The structure was solved by direct methods through the weighted numerical addition procedure and refined by block-diagonal least squares. The final conventional R factor is 0.044. The mol. lies on a crystallog. center of symmetry. The central pyran rings have boat conformation with their 4 H atoms trans to each other. The Ph and pyran rings have a dihedral angle of 87.9°. Packing is consistent with van der Waals interactions.

IT 54497-37-9

RL: PRP (Properties)

(crystal structure of)

RN 54497-37-9 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran, 4b,5,10b,11-tetrahydro-1,3,7,9-tetramethyl-5,11-diphenyl-, (4b $\alpha$ ,5 $\alpha$ ,10b $\beta$ ,11 $\beta$ )- (9CI)  
(CA INDEX NAME)

~~L22~~ ANSWER 44 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1973:526351 CAPLUS

DOCUMENT NUMBER: 79:126351

TITLE: One-step synthesis of coumarino(3,4:4',3')isocoumarins

AUTHOR(S): Darbarwar, Malleshwar; Sundaramurthy, V.; Rao, N. V. Subba

CORPORATE SOURCE: Dep. Chem., Osmania Univ., Hyderabad, India

SOURCE: Indian Journal of Chemistry (1973), 11(7), 637-40

CODEN: IJOCAP; ISSN: 0019-5103

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The condensation of the sodium salt of 4-hydroxycoumarin and 2-BrC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H in aqueous solution under the catalytic influence of CuSO<sub>4</sub> gave coumarino[3,4:4',3']isocoumarin (I) on the basis of uv, ir, and mass spectra. The general applicability of the reaction was established.

IT 2288-98-4P 27284-76-0P 27284-77-1P

27284-78-2P 27284-79-3P 27284-80-6P

49634-80-2P 49634-81-3P 49634-82-4P

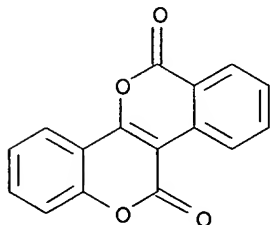
49634-83-5P 49634-84-6P 49634-85-7P

49634-86-8P 49634-87-9P 49686-95-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

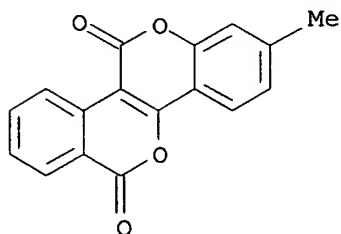
RN 2288-98-4 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione (8CI, 9CI) (CA INDEX NAME)



RN 27284-76-0 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 2-methyl- (8CI, 9CI)  
(CA INDEX NAME)

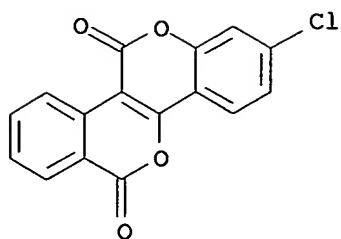


RN 27284-77-1 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 2-chloro- (8CI, 9CI)  
(CA INDEX NAME)

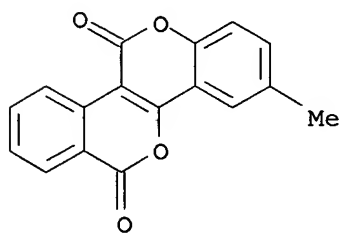


10/307,735



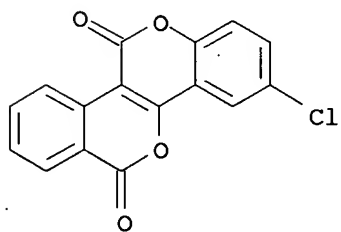
RN 27284-78-2 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 3-methyl- (8CI, 9CI)  
(CA INDEX NAME)



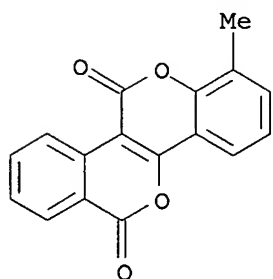
RN 27284-79-3 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 3-chloro- (8CI, 9CI)  
(CA INDEX NAME)



RN 27284-80-6 CAPLUS

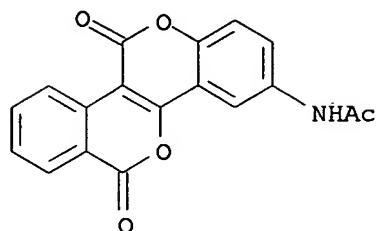
CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 1-methyl- (8CI, 9CI)  
(CA INDEX NAME)



RN 49634-80-2 CAPLUS

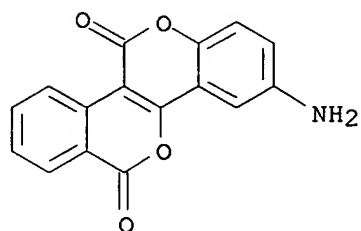
10/307,735

CN Acetamide, N-(6,11-dioxo-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-3-yl)-  
(9CI) (CA INDEX NAME)



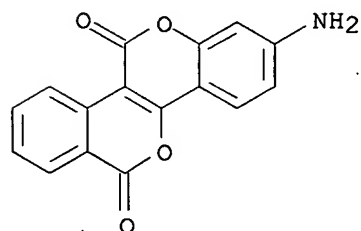
RN 49634-81-3 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 3-amino- (9CI) (CA  
INDEX NAME)



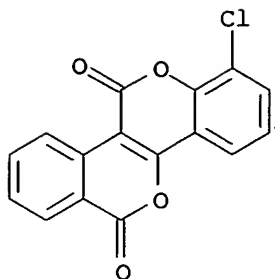
RN 49634-82-4 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 2-amino- (9CI) (CA  
INDEX NAME)



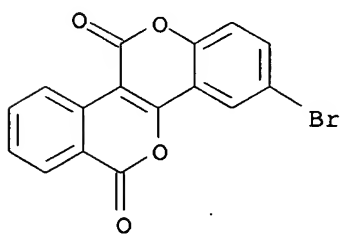
RN 49634-83-5 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 1-chloro- (9CI) (CA  
INDEX NAME)



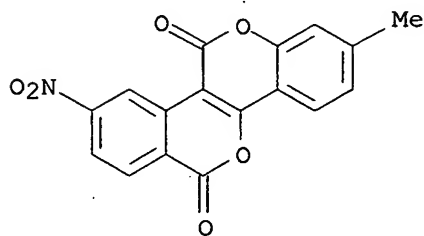
RN 49634-84-6 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 3-bromo- (9CI) (CA INDEX NAME)



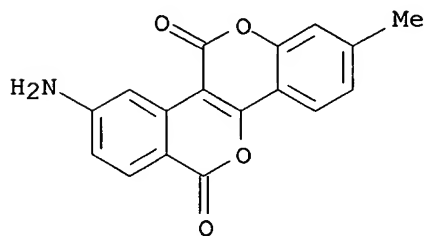
RN 49634-85-7 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 2-methyl-9-nitro- (9CI) (CA INDEX NAME)



RN 49634-86-8 CAPLUS

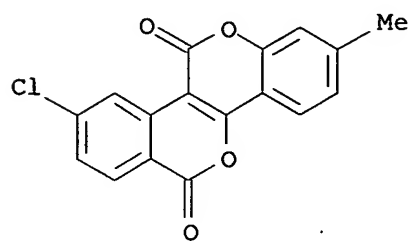
CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 9-amino-2-methyl- (9CI) (CA INDEX NAME)



10/307,735

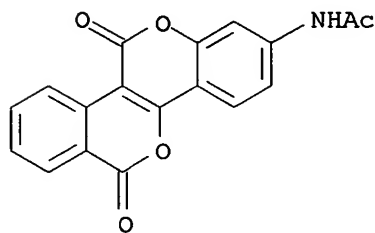
RN 49634-87-9 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 9-chloro-2-methyl-  
(9CI) (CA INDEX NAME)



RN 49686-95-5 CAPLUS

CN Acetamide, N-(6,11-dioxo-6H,11H-[2]benzopyrano[4,3-c][1]benzopyran-2-yl)-  
(9CI) (CA INDEX NAME)



L22 X ANSWER 45 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1972:514640 CAPLUS

DOCUMENT NUMBER: 77:114640

TITLE: Heterocyclic steroids. XXV. Total synthesis of modified 6-thiaestrogens

AUTHOR(S): Koenst, W. M. B.; Van Bruynsvoort, Mrs. J.; Speckamp, W. N.; Huisman, H. O.

CORPORATE SOURCE: Lab. Org. Chem., Univ. Amsterdam, Amsterdam, Neth.

SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1972), 91(7), 869-82

CODEN: RTCPA3; ISSN: 0165-0513

DOCUMENT TYPE: Journal

LANGUAGE: English

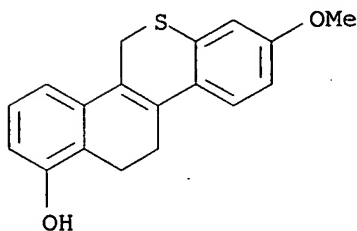
AB 6-Thiasteroids have been totally synthesized by the reaction of 2-substituted 1,3-cyclopentanediones with 4-hydroxy-4-vinylthiochromans or with the derived isothiuronium salts. Modifications of the C-13 substituent have also been carried out via the T1 salt of the 18-nor-8,14-secosteroid. When using 2-chloro- and 2-acetylamino-1,3-cyclopentanediones anomalous reaction products were obtained.

IT 28105-10-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 28105-10-4 CAPLUS

CN 5H-Benzo[b]naphtho[2,1-d]thiopyran-1-ol, 11,12-dihydro-8-methoxy- (8CI, 9CI) (CA INDEX NAME)



~~L22~~ ANSWER 46 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1971:87870 CAPLUS

DOCUMENT NUMBER: 74:87870

TITLE: New route to dehydrorotenone and other rotenoids

AUTHOR(S): Baran-Marszak, Maurice; Massicot, Jacques; Molho, Darius

CORPORATE SOURCE: Lab. Chim. Appl. Corps Organise, Museum Natl. Hist. Nat., Paris, Fr.

SOURCE: Bulletin de la Societe Chimique de France (1971), (1), 191-8

CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal

LANGUAGE: French

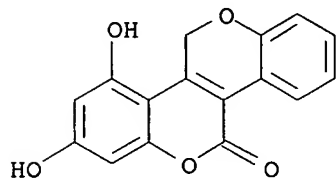
AB The thermal condensation of alkyl 3-chromanone-4-carboxylates with phenols resulted in dehydrorotenoids. The condensation of 6,7-methoxy-4-(ethoxycarbonyl)-3-chromanone with tubanol gave dehydrorotenone. Also prepared were dehydromunduserone, de-hydrosermundone, and dehydroapotoxicarol.

IT 30990-38-6P 30990-39-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

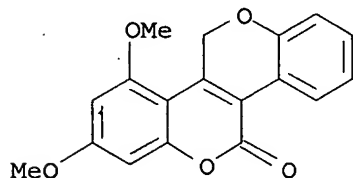
RN 30990-38-6 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5(11H)-one, 8,10-dihydroxy- (8CI) (CA INDEX NAME)

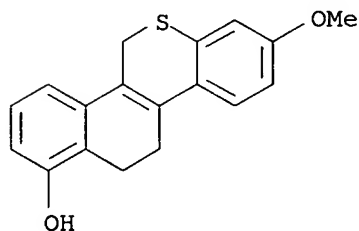


RN 30990-39-7 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5(11H)-one, 8,10-dimethoxy- (8CI) (CA INDEX NAME)



~~L2~~ ANSWER 47 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1970:456292 CAPLUS  
DOCUMENT NUMBER: 73:56292  
TITLE: Heterocyclic steroids. XVII. Anomalous spiro- and aromatized 6-thiaestrogens  
AUTHOR(S): Koenst, W. M. B.; Van-Bruynsvoort, Mrs. J. L.; Speckamp, Willem N.; Huisman, Henderikus O.  
CORPORATE SOURCE: Lab. Org. Chem., Univ. Amsterdam, Amsterdam, Neth.  
SOURCE: Tetrahedron Letters (1970), (29), 2527-30  
CODEN: TELEAY; ISSN: 0040-4039.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI For diagram(s), see printed CA Issue.  
AB Reaction of I with II (from III) in Me<sub>2</sub>CHOH-H<sub>2</sub>O gave IV, which was cyclized (HCl-dioxane) to V. On recrystn. of V from MeOH, V gave VI, which was dehydrated by HCl-dioxane to VII. Analogous reaction series starting with VIII and II gave IX which was cyclized (HCl-dioxane) to give X. Aromatization of X with acid gave XI. The reaction of III and XII in xylene or MeNO<sub>2</sub> at 120° gave XIII, while the reaction at 90° gave XIV. III and XV in refluxing MeNO<sub>2</sub> gave XVI.  
IT **28105-10-4P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
RN 28105-10-4 CAPLUS  
CN 5H-Benzo[b]naphtho[2,1-d]thiopyran-1-ol, 11,12-dihydro-8-methoxy- (8CI, 9CI) (CA INDEX NAME)



122 ANSWER 48 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1970:121394 CAPLUS

DOCUMENT NUMBER: 72:121394

TITLE: Synthesis of coumarino[3,4:2',3']isocoumarins

AUTHOR(S): Darbarwar, Malleshwar; Sundaramurthy, V.; Rao, Nandury V. S.

CORPORATE SOURCE: Dep. Chem., Osmania Univ., Hyderabad, India

SOURCE: Indian Journal of Chemistry (1970), 8(2), 197-8

CODEN: IJOCAP; ISSN: 0019-5103

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB A number of substituted 4-hydroxycoumarins have been condensed with o-bromobenzoic acid in alkaline medium under the catalytic influence of aqueous CuSO<sub>4</sub>. The compds. obtained have been characterized as coumarino-[3,4:2',3']isocoumarins (I, R = Me, Cl) on the basis of ir and mass spectral data.

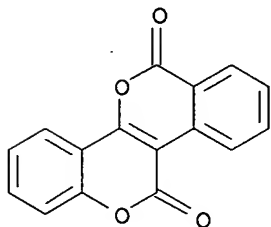
IT 2288-98-4P 27284-76-0P 27284-77-1P

27284-78-2P 27284-79-3P 27284-80-6P

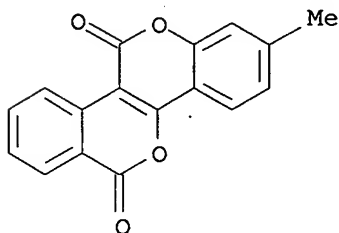
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 2288-98-4 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione (8CI, 9CI) (CA INDEX NAME)



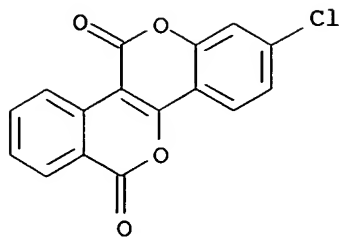
RN 27284-76-0 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 2-methyl- (8CI, 9CI)  
(CA INDEX NAME)

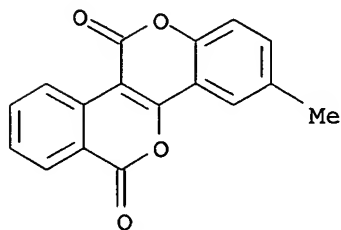
RN 27284-77-1 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 2-chloro- (8CI, 9CI)  
(CA INDEX NAME)

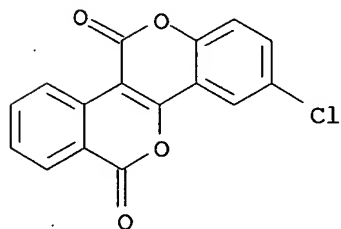




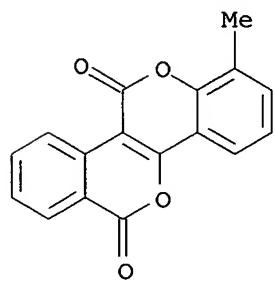
RN 27284-78-2 CAPLUS  
 CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 3-methyl- (8CI, 9CI)  
 (CA INDEX NAME)



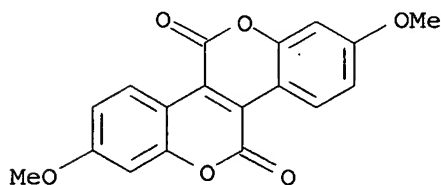
RN 27284-79-3 CAPLUS  
 CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 3-chloro- (8CI, 9CI)  
 (CA INDEX NAME)



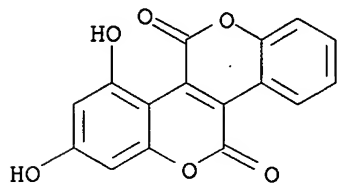
RN 27284-80-6 CAPLUS  
 CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione, 1-methyl- (8CI, 9CI)  
 (CA INDEX NAME).



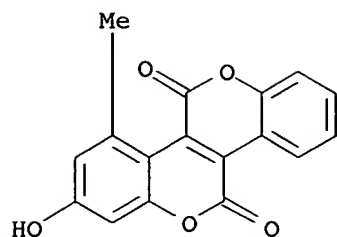
~~L22~~ ANSWER 49 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1968:496520 CAPLUS  
 DOCUMENT NUMBER: 69:96520  
 TITLE: Dibenzonaphthyrone and related compounds  
 AUTHOR(S): Chatterjea, J. N.; Prasad, N.  
 CORPORATE SOURCE: Patna Univ., Patna, India  
 SOURCE: Journal of the Indian Chemical Society (1968), 45(1), 35-44  
 CODEN: JICSAH; ISSN: 0019-4522  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI For diagram(s), see printed CA Issue.  
 AB New syntheses of dibenzonaphthyrone (I) have been carried out from 2,2-dimethoxysuccinonitrile and trans-2,2-dimethoxydicyanostilbene. Several derivs. of dibenzonaphthyrone have been synthesized from 3-(2-methoxyphenyl)-4-ethoxycarbonylcoumarins prepared by the method of Borsche and Wannagat (1950). The structures have been confirmed by independent conventional syntheses. Borsche and Wannagat's synthesis of 3-phenylcoumarin-4-carboxylic acid has been extended to show that if  $\alpha$ -acetylphenylacetonitrile is employed in place of Et phenylcyanopyruvate, good yields of 3-phenyl-4-methylcoumarins are obtained.  
 IT 20503-13-3P 20503-15-5P 20503-18-8P  
 20589-90-6P 20589-91-7P 20752-64-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 20503-13-3 CAPLUS  
 CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 2,8-dimethoxy- (8CI) (CA INDEX NAME)



RN 20503-15-5 CAPLUS  
 CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 2,4-dihydroxy- (8CI, 9CI) (CA INDEX NAME)

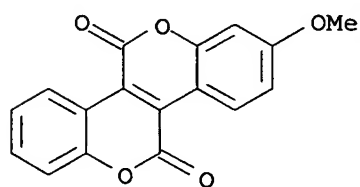


RN 20503-18-8 CAPLUS  
 CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 2-hydroxy-4-methyl- (8CI) (CA INDEX NAME)



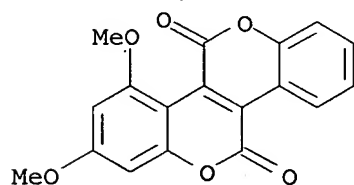
RN 20589-90-6 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 2-methoxy- (8CI) (CA INDEX NAME)



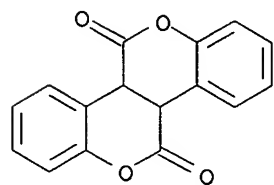
RN 20589-91-7 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 2,4-dimethoxy- (8CI) (CA INDEX NAME)



RN 20752-64-1 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 4b,10b-dihydro- (8CI) (CA INDEX NAME)



~~122~~ ANSWER 50 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1967:18650 CAPLUS

DOCUMENT NUMBER: 66:18650

TITLE: Structure of flavanonol-red

AUTHOR(S): Kubota, Takashi; Ichikawa, Nobutaka; Matsuo, K.;  
Shibata, Kazuhiro

CORPORATE SOURCE: City Univ. Osaka, Osaka, Japan

SOURCE: Tetrahedron Letters (1966), (39), 4671-4

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

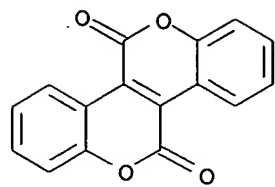
AB cf. CA 36, 41188. Flavanonols (flavanonol, m. 208-10°; 4'-bromo-3-hydroxyflavanone, m. 299-300°; ampeloptin, m. 223-4°) boiled with Ac<sub>2</sub>O and NaOAc gave a series of red pigments. Similar treatment of 3-hydroxyflavanone gave the title compound (I), hydrogenated in dioxane over prerduced PtO<sub>2</sub> with 3 moles H to a hexahydro compound (II), m. 183-4°, showing no HO, AcO, or CO absorption in the ir spectrum. Ozonization of I followed by reductive decomposition gave PhCH<sub>2</sub>OH and o-HOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H. Hydrogenolysis of I with Na-liquid NH<sub>3</sub> according to Tomita, et al. (CA 46, 5060g) gave a dihydroxy compound (III), C<sub>30</sub>H<sub>26</sub>O<sub>3</sub>, m. 154-5°; diacetate, m. 110-12°. I heated 1 hr. in AcOH containing H<sub>2</sub>SO<sub>4</sub> gave a good yield of a dioxo-diphenol (IV, R = H) (V), m. 211-12° (decomposition), pos. test with ferricyanide and ferric salts; diacetate IV (R = Ac) (VI), m. 162.5-3.0°; di-Me ether IV (R = Me) (VII), m. 194-5°. V boiled in Ac<sub>2</sub>O-NaOAc did not regenerate I but only formed VI. Catalytic reduction of VI over Pd-C gave III diacetate. Catalytic reduction of VII gave a tetrahydro derivative, m. 99-100°, showing no ir OH or CO absorption. Reduction of VII with NaBH<sub>4</sub> in boiling dioxane-MeOH gave a dihydroxydimethyl ether, m. 178-9° (decomposition),  $\nu$  3300 cm.<sup>-1</sup> (no absorption at 1660 or 880 cm.<sup>-1</sup>) also obtained by reduction of VII with LiAlH<sub>4</sub> in the cold. Ozonolysis of VII gave BzOH and a yellow crystalline anhydride (VIII, R = Me), m. 159-60°, identifying the compound as bis(o-methoxyphenyl)maleic anhydride, also synthesized from o-MeOC<sub>6</sub>H<sub>4</sub>CHO. The data suggested the assigned formulation for I and its derivs. but do not exclude the alternative formula (IX). I in EtOAc irradiated with sunlight or uv light in air at 20° gave green crystalline photoflavanol-red (X), m. 218-20°, hydrolyzed in alkali to give equimolar amts. of BzOH and a hydroxy compound (XI, R = H) (XII), m. 275-80°, reconverted to X by benzoylation. XII treated with Me<sub>2</sub>SO<sub>4</sub> and K<sub>2</sub>CO<sub>3</sub> in anhydrous Me<sub>2</sub>CO gave the monomethyl ether XI (R = Me) (XIII), m. 182-3°. XII oxidized with KMnO<sub>4</sub>-Me<sub>2</sub>CO or by air in a mixture of aqueous NaOH, tetrahydrofuran, and alc. under reflux gave BzOH and the known (Chovin, CA 37, 27371) dilactone (XIV), m. 295-6°. XIII was ozonized to give BzOMe and the anhydride VIII (R = H), m. 160-1°,  $\nu$  760 cm.<sup>-1</sup>, converted to VIII (R = Me) by methylation with alkaline Me<sub>2</sub>SO<sub>4</sub>. Formation of BzOMe in the ozonolysis of XIII excluded the alternative formulation IX but all the above reactions supported the assigned formula I.

IT 13225-81-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 13225-81-5 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione (8CI, 9CI) (CA INDEX NAME)



~~L72~~ ANSWER 51 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1965:439038 CAPLUS

DOCUMENT NUMBER: 63:39038

ORIGINAL REFERENCE NO.: 63:6981f-h

TITLE: Isocoumarino[3,4:4',3']coumarin

AUTHOR(S): Chatterjea, J. N.; Banerjee, B. K.; Prasad, N.

CORPORATE SOURCE: Sci. Coll., Patna

SOURCE: J. Indian Chem. Soc. (1965), 42(5), 283-8

DOCUMENT TYPE: Journal

LANGUAGE: English

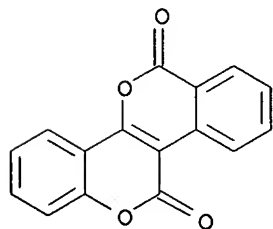
GI For diagram(s), see printed CA Issue.

AB I [R = o-MeOC<sub>6</sub>H<sub>4</sub>, R' = CN (II)] (0.1 g.) and 1 g. C<sub>5</sub>H<sub>5</sub>N.HCl heated at 210-20° for 1 hr. under CO<sub>2</sub> gave quant. III [A = O (IV)], m. 282° (AcOH),  $\lambda$  5.72 and 5.89  $\mu$  (C:O). IV heated with MeOH-NH<sub>3</sub> for 30 hrs. at 100° produced III (A = NH), m. 310°. The preparation of II, m. 175-6°, represented an extension of the isocoumarin synthesis of Chatterjea (CA 48, 7003d), and was obtained by refluxing 1.3 g. o-NCCH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Me, 1.6 g. o-MeOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Et, 0.23 g. NaH, and 40 ml. anhydrous C<sub>6</sub>H<sub>6</sub> for 18 hrs. Other I derivs. prepared were as follows (R, R', and m.p. given): H, CN, 156°; H, CO<sub>2</sub>H, 250°; H, H, -; C<sub>2</sub>Et, CN, 173°; CO<sub>2</sub>H, H, 243°; Ph, CN, 205°. In an attempt to prepare the dimer of bicyclo[4.2.0]octa-1,3,5-triene 7,8-dione (V) isolated by Cava, et al. (CA 59, 3843e), o-OCHC<sub>6</sub>H<sub>4</sub>-CO<sub>2</sub>Me was treated with KCN-EtOH and found to give not V but  $\Delta$ 3,3'-bipthalide (VI). Both V and VI treated with alkali produced 3-hydroxy-3,3'-bipthalide. Me opianate in a min. quantity of 50% EtOH warmed 30 min. with KCN gave 6,6',7,7'-tetramethoxy- $\Delta$ 3,3'-bipthalide, m. 305°.

IT 2288-98-4,  $\alpha$ ,2-Stilbenedicarboxylic acid,  
 $\alpha'$ ,2'-dihydroxy-, di- $\delta$ -lactone  
 (preparation of)

RN 2288-98-4 CAPLUS

CN 6H,11H-[2]Benzopyrano[4,3-c][1]benzopyran-6,11-dione (8CI, 9CI) (CA INDEX NAME)



122 ANSWER 52 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1965:74100 CAPLUS  
DOCUMENT NUMBER: 62:74100  
ORIGINAL REFERENCE NO.: 62:13115e-h,13116a-b  
TITLE: Cyclic condensation of homophthalic acid dimethyl ester with  $\alpha,\beta$ -unsaturated carbonyl compounds

AUTHOR(S): Eisenhuth, W.; Renfro, H. B.; Schmid, H.  
CORPORATE SOURCE: Univ. Zurich, Switz.  
SOURCE: Helvetica Chimica Acta (1965), 48(2), 375-9  
CODEN: HCACAV; ISSN: 0018-019X

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 62:74100

GI For diagram(s), see printed CA Issue.

AB o-C<sub>6</sub>H<sub>4</sub>(CH<sub>2</sub>CO<sub>2</sub>Me)CO<sub>2</sub>Me (I) (395 mg.) and 220 mg. MeCH:CHCO<sub>2</sub>Me was heated 4 hrs. at 95° in 1 ml. absolute MeOH containing 92 mg. Na and worked up to give 240 mg. II (R = Me), m. 52-60° (Et<sub>2</sub>O-C<sub>5</sub>H<sub>12</sub> at -20°); it gave a deep violet FeCl<sub>3</sub> color reaction. Similarly, 219 mg. I, 159 mg. di-Me maleate and 51 mg. Na in 1 ml. MeOH kept overnight gave 179 mg. II (R = CO<sub>2</sub>Me), m. 118-20° (Et<sub>2</sub>O). I and PhCH:CHCO<sub>2</sub>Me gave 55.5% II (R = Ph), m. 121-31° (CH<sub>2</sub>Cl<sub>2</sub>-C<sub>5</sub>H<sub>12</sub>); FeCl<sub>3</sub> reaction violet. I (1.07 g.), 787 mg. coumarin, and 302 mg. Na in 3 ml. MeOH 8 hrs. at 90-5° gave 39% III, m. 140-70° (CH<sub>2</sub>Cl<sub>2</sub>-Et<sub>2</sub>O); FeCl<sub>3</sub> reaction red violet. Acidification of the reaction mixture sometimes gave a product, m. 178-81°, which on distillation in high vacuum gave III. III (200 mg.) and 1 g. chloranil in 4 ml. PhMe heated 6 hrs. at 145°, or in 4 ml. xylene 2.5 hrs. at 160°, and sublimation (170-200°) of the residue of the evaporated solution gave 83% IV (R = CO<sub>2</sub>Me, R' = H) (V), m. 211-12° (CH<sub>2</sub>Cl<sub>2</sub>-EtOH); FeCl<sub>3</sub> color in HCONMe<sub>2</sub>-H<sub>2</sub>O dark green. V (1.35 g.), 5 ml. MeI, and 6.5 g. K<sub>2</sub>CO<sub>3</sub> in 50 ml. dry Me<sub>2</sub>CO refluxed 15 hrs. with the addition of another 5 ml. MeI after 7 hrs. gave 85.2% IV (R = CO<sub>2</sub>Me, R' = Me) (VI), m. 162-4° (CH<sub>2</sub>Cl<sub>2</sub>-Et<sub>2</sub>O). V (54 mg.) warmed slightly with 2 ml. concentrated H<sub>2</sub>SO<sub>4</sub>, and

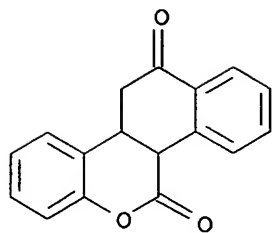
the

mixture kept 0.5 hr. at 20° and poured onto ice gave 44.5% IV (R = R' = H) (VII), yellow-green, m. 206-7° (CH<sub>2</sub>Cl<sub>2</sub>-Et<sub>2</sub>O); FeCl<sub>3</sub> color in EtOH deep green. VII was also obtained in 80.5% yield by heating 103 mg. III with 3.5 ml. polyphosphoric acid (PPA). VI heated 9 hrs. with PPA at 100-5° gave VII. III (103 mg.) was kept in excess 3% KOH in 1:1 MeOH-H<sub>2</sub>O containing a small amount Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub> 20 hrs. at 20° under N, and the solution adjusted to pH .apprx.1, kept 3 hrs., and worked up to give 72.2% VIII, b0.01 150-70°, m. 185-6° (CH<sub>2</sub>Cl<sub>2</sub>-Et<sub>2</sub>O). VIII was also formed in 95.5% yield when 213 mg. III was refluxed 3 days with anhydrous HCO<sub>2</sub>H. Condensation of 350 mg. I with 328 mg. 1-methyl-2-quinolone in 1.5 ml. iso-PrOH containing 147 mg. K 15 hrs. at 100° gave 32% IX, m. 226-9°. Pertinent uv, ir, and N.M.R. spectral data were given.

IT 734-48-5, 1-Naphthoic acid, 1,2,3,4-tetrahydro-2-(o-hydroxyphenyl)-4-oxo-,  $\delta$ -lactone (preparation of)

RN 734-48-5 CAPLUS

CN 1-Naphthoic acid, 1,2,3,4-tetrahydro-2-(o-hydroxyphenyl)-4-oxo-,  $\delta$ -lactone (7CI, 8CI) (CA INDEX NAME)





L22 ANSWER 53 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1962:462484 CAPLUS

DOCUMENT NUMBER: 57:62484

ORIGINAL REFERENCE NO.: 57:12377f-h

TITLE: Condensation of some oxo esters with 2,4- and 2,6-xlenols

AUTHOR(S): Smith, Robert V.; Bealor, Mark D.

CORPORATE SOURCE: S. C. Johnson &amp; Son, Inc., Racine, WI

SOURCE: Journal of Organic Chemistry (1962), 27, 3092-6

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

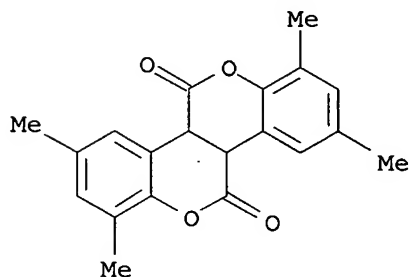
AB The condensation of several oxo dibasic acid esters with 2,4- and 2,6-xlenols in cold concentrated H<sub>2</sub>SO<sub>4</sub> was carried out. In the case of 2,6-xlenol, the corresponding bisphenol acids or esters were obtained with the exception of diethyl  $\alpha$ -oxoglutarate, where two products were isolated,  $\alpha$ -(3,5-dimethyl-4-hydroxyphenyl)glutaconic anhydride and  $\alpha,\alpha$ -bis(3,5-dimethyl-4-hydroxyphenyl)glutaric anhydride. With 2,4-xlenol, several lactones were formed. A spirodilactone was isolated from diethyl  $\alpha$ -oxosuccinate. A non-spirodilactone, resulting from rearrangement, was formed from diethyl  $\alpha$ -oxoglutarate. Structural assignments are based on elemental, infrared, and nuclear magnetic resonance.

IT 94549-82-3, Succinic acid, 2,3-bis(2-hydroxy-3,5-xyllyl)-, di- $\delta$ -lactone

(preparation of)

RN 94549-82-3 CAPLUS

CN Succinic acid, 2,3-bis(2-hydroxy-3,5-xyllyl)-, di- $\delta$ -lactone (7CI)  
(CA INDEX NAME)



122 ANSWER 54 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1961:87402 CAPLUS  
 DOCUMENT NUMBER: 55:87402  
 ORIGINAL REFERENCE NO.: 55:16502c-i,16503a-e  
 TITLE: Ozonolysis of polycyclic hydrocarbons. II  
 AUTHOR(S): Copeland, P. G.; Dean, R. E.; McNeil, D.  
 CORPORATE SOURCE: Coal Tar Research Assoc., Gomersal, UK  
 SOURCE: Journal of the Chemical Society, Abstracts (1961)  
 1232-8  
 CODEN: JCSAAZ; ISSN: 0590-9791  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 OTHER SOURCE(S): CASREACT 55:87402

AB cf. CA 55, 1555h. The ozonolysis of phenanthrene (I), chrysene (II), picene (III), benzo[g]chrysene (IV), dibenzo[*cg*]phenanthrene (V), triphenylene (VI), and benz[*a*]anthracene (VII) was described. In each case, O<sub>3</sub> attacked the bond(s) possessing the lowest bond localization energy. Improved preps. of these hydrocarbons were also reported. I (1.78 g.) in 60 ml. CCl<sub>4</sub> treated at -20° with an equimolar amount of O<sub>3</sub>, and the ozonide purified via CHCl<sub>3</sub>-ligroine gave a product, m. 131-2°. The crude ozonide (1.78 g.) in 50 ml. H<sub>2</sub>O and 50 ml. C<sub>5</sub>H<sub>5</sub>N at 60-5° treated with 6.5 g. KMnO<sub>4</sub> gave 81% diphenic acid (VIII), m. 230-1°. In another experiment, the crude ozonide from 1.78 g. I kept 12 hrs. in 50 ml. H<sub>2</sub>O and 50 ml. C<sub>5</sub>H<sub>5</sub>N gave 2,2'-diformylbiphenyl, isolated in 34% yield as the dioxime, prisms, m. 180° (aqueous alc.). Oxidation of 1.78 g. I gave 34% unchanged I, 51% phenanthraquinone, and 5% VIII. With C<sub>5</sub>H<sub>5</sub>N as the solvent (at 0°) about 1.7 moles O<sub>3</sub> was required. Permanganate decomposition gave 74% crude VIII. Ozonolysis of 3.56 g. I in 60 ml. (Cl<sub>2</sub>CH)<sub>2</sub> at 0°, followed by treatment (1 hr.) with 15 ml. 30% H<sub>2</sub>O<sub>2</sub> and 50 ml. 10% NaOH gave 2.82 g. of an alkali-insol. residue. Acidification of the filtrate gave 0.65 g. crude VIII. II, m. 254-5°, (2.28 g.) in (Cl<sub>2</sub>CH)<sub>2</sub> similarly treated with O<sub>3</sub> gave 1.4 g. 2-(*o*-carboxyphenyl)-1-naphthoic acid (IX), m. 213-14° (10% HCl); di-Me ester, prisms, m. 93-4°. Decarboxylation of IX with soda-lime gave 71% 2-phenylnaphthalene, m. 101-2°. Treatment of 2.28 g. II with KMnO<sub>4</sub> in C<sub>5</sub>H<sub>5</sub>N gave 2.05 g. II and 0.17 g. chrysene-5,6-quinone (X). Decomposition of II ozonide with alkaline H<sub>2</sub>O<sub>2</sub> gave

an

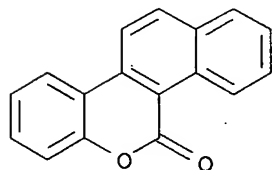
alkali-insol. resin and no pure acid. II (7.25 g.) in 1200 ml. AcOH at 85-90° treated 3 hrs. with 40 ml. 30% H<sub>2</sub>O<sub>2</sub>, the mixture stirred 5 hrs. at 90°, and the alkali-insol. material chromatographed on Al<sub>2</sub>O<sub>3</sub> gave 1.15 g. unchanged II and 0.63 g. 2-(*o*-hydroxyphenyl)-1-naphthoic acid lactone (XI), m. 191° (C<sub>6</sub>H<sub>6</sub>). Acidification of the alkaline extract gave 2.9 g. IX. X was prepared in 57% yield by oxidation of

II with

Na<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> in AcOH. Oxidation of 5 g. X with H<sub>2</sub>O<sub>2</sub> in AcOH gave 0.53 g. XI and 2.9 g. dicarboxylic acid. III was obtained in 21% yield as plates, m. 365° (C<sub>5</sub>H<sub>5</sub>N), by the cyclization of 1,2-di- $\alpha$ -naphthylethane (XII) with AlCl<sub>3</sub>. XII was prepared as follows: MeMgI (from 120 g. MeI) and 124 g. 1-chloromethylnaphthalene in 250 ml. Et<sub>2</sub>O refluxed 1.5 hrs. gave (after an addnl. 2 hrs. of reflux) 57.5 g. XII, m. 162-3° (alc.-C<sub>6</sub>H<sub>6</sub>). III (2.78 g.) in 60 ml. (Cl<sub>2</sub>CH)<sub>2</sub> similarly ozonized gave 1.35 g. p-terphenyl-2,2',3',2''-tetracarboxylic acid 2',3'-anhydride (XIII), m. 284-6° (decomposition) (aqueous Me<sub>2</sub>CO). Decarboxylation of XIII with soda lime gave 67% terphenyl, m. 210°; di-Me ester of XIII, m. 207°. Chromatography of the mother liquor from this ester on Al<sub>2</sub>O<sub>3</sub> gave the tetramethyl ester, m. 115° (ligroine). When 1.39 g. III was treated with an equimolar amount of O<sub>3</sub>, 44% III was recovered and 9%

XIII isolated. Benzo[g]chrysene-11,12-dicarboxylic anhydride (3.3 g.), 3.3 g. Cu powder, and 25 ml. quinoline refluxed 2 hrs. and the residue chromatographed on Al<sub>2</sub>O<sub>3</sub> gave 1.45 g. IV, m. 116° (AcOH). Cyclization of 1.9 g. 1',2-epoxide from 1-(2-biphenyl)-3,4-dihydronaphthalene with HBr in AcOH gave 1.3 g. 11,12-dihydrobenzo[g]chrysene (XIV), m. 136-7°. XIV (8.7 g.) dehydrogenated during 24 hrs. with 2 g. 10% Pd-C in 150 ml. p-cymene in a stream of CO<sub>2</sub> gave 7.8 g. IV. IV (2.78 g.) in 60 ml. (Cl<sub>2</sub>CH)<sub>2</sub> at 0° treated with O<sub>3</sub> gave 69% 10-(o-carboxyphenyl)phenanthrene-9-carboxylic acid (XV), m. 286° (decomposition); di-Me ester m. 173° (MeOH). Decarboxylation of XV with Cu powder gave 70% 9-phenylphenanthrene, m. 105°. 3,3',4,4'-Tetrahydro-1,1'-binaphthyl was converted to V. The final stage was improved as follows: a slow stream of CO<sub>2</sub> passed during 2 days through a mixture of 1,2,7,8-tetrahydrodibenzo[*cg*]phenanthrene (7.27 g.), 2.5 g. 10% Pd-C, and 150 ml. p-cymene and the residue chromatographed on Al<sub>2</sub>O<sub>3</sub> gave 4.12 g. V, prisms, m. 181-2°, and 1.54 g. benzo[ghi]perylene, yellow prisms, m. 280-1° (xylene). V (2.78 g.) similarly ozonized gave 2.64 g. o-terphenyl-2,2'',3',6'-tetracarboxylic acid (XVI), m. 302° (decomposition); tetramethyl ester m. 125° (ligroine). Decarboxylation of XVI with soda lime gave 14.5% VI, m. 199°, whereas Cu and quinoline gave 60% o-terphenyl, m. 57°. Distillation of o-terphenyl with soda lime gave 5% VI. VI (2.28 g.) similarly ozonized at 0° gave 22% phenanthrene-9,10-dicarboxylic acid anhydride, m. 315-16°. The acidic filtrate gave 0.19 g. VIII. Decomposition of the ozonide with alkaline peroxide gave the anhydride and VIII in similar yield. Absorption of 3 or 4 moles O<sub>3</sub> led to resins, from which 16% and 20% VIII was isolated. VII (2.28 g.) similarly ozonized and the product chromatographed gave 28% unchanged VII and 13% benz[a]anthracene-7,12-quinone (XVII), m. 169°. Decomposition of the ozonide with KMnO<sub>4</sub> in aqueous C<sub>5</sub>H<sub>5</sub>N and acidification of the alkaline liquor gave 0.24 g. 3-(o-carboxyphenyl)-2-naphthoic acid (XVIII), m. 250° (10% HCl); di-Me ester, rhombs, m. 87°. Decarboxylation of XVIII with soda lime gave 66% 2-phenylnaphthalene, m. 101-2°. Absorption of 2 moles O<sub>3</sub> by VII gave 17% each XVII and XVIII. Absorption of 3 moles O<sub>3</sub> afforded an ozonide, which decomposed spontaneously when dried. VII (2.28 g.) treated with 1 mole O<sub>3</sub> and the ozonide decomposed with alkaline peroxide gave 0.72 g. VII and 21.6% XVII. VII (5 g.) oxidized in AcOH with 30% H<sub>2</sub>O<sub>2</sub> and the alkali insol. material chromatographed on activated Al<sub>2</sub>O<sub>3</sub> gave 2.1 g. XVII and 1.31 g. XVIII. XVII (2.58 g.) in 60 ml. CHCl<sub>3</sub> at -20° treated with 20 millimoles O<sub>3</sub>, then treated with alkaline H<sub>2</sub>O<sub>2</sub>, heated 1 hr. at 60°, and the product isolated gave 2.37 g. anthraquinone-1,2-dicarboxylic acid, m. 320-2° (H<sub>2</sub>O); di-Me ester, yellow prisms, m. 210-11° (EtOAc). The acid yielded 91% anthraquinone on decarboxylation with Cu.

IT 4708-17-2, 1-Naphthoic acid, 2-(o-hydroxyphenyl)-,  $\delta$ -lactone  
(preparation of)  
RN 4708-17-2 CAPLUS  
CN 5H-Benzo[b]naphtho[2,1-d]pyran-5-one (8CI, 9CI) (CA INDEX NAME)



~~L22~~ ANSWER 55 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1960:2218 CAPLUS

DOCUMENT NUMBER: 54:2218

ORIGINAL REFERENCE NO.: 54:518b-i,519a

TITLE: Synthesis of furano compounds. XV. 3-Acylisocoumaranones and the rearrangement of their phenylhydrazones

AUTHOR(S): Chatterjea, J. N.

CORPORATE SOURCE: Sci. Coll., Patna

SOURCE: J. Indian Chem. Soc. (1959), 36, 69-75

DOCUMENT TYPE: Journal

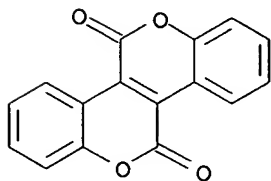
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

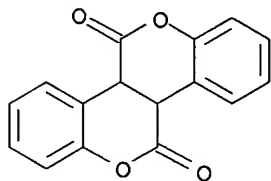
AB cf. C.A. 53, 15037e. It has been shown that the phenylhydrazones of 3-acylisocoumaranones, like those of thiooxindoles (Glauert and Mann, C.A. 47, 1129i) and 3-acylindoles (Alberti, C.A. 42, 2963i), underwent rearrangement to the related pyrazolones by the action of HCl or heat. The acylisocoumaranones were prepared by the action of N,N'-diarylamidines on isocoumaranone (I) or by the direct Gattermann synthesis with I (G. and M., C.A. 47, 1125g). I (1.0 g.) with 1.4 g. diphenylformamide gave 1.4 g. yellow anil (II), m. 160-1°. II (2.5 g.) boiled with 20 cc. 10% NaOH yielded 0.85 g. 3-formylcoumaran-2-one (III), m. 169 (dilute EtOH); phenyl hydrazone, cream colored from alc., m. 176° (quick heating) was converted at m. p. or by boiling 2-3 hrs. with alc. HCl (10%) to 4-o-hydroxyphenyl-1-phenylpyrazol-5-one, m. 233° (EtOH). II (0.4 g.) boiled 4 hrs. with a mixture of 3 cc. HOAc and 0.3 cc. HCl, gave 0.1 g. coumarone. Similarly, 1.0 g. I and 1.5 g. diphenylacetamide gave 1.1 g. anil as needles (EtOH), m. 134°, converted to 0.55 g. 3-acetylisocoumaranone, m. 135-6° (dilute EtOH); phenylhydrazone (IV), colorless leaflets, m. 170°. I (0.5 g.) and 0.75 g. N,N'-diphenylbenzamide gave 0.5 g. anil (V), m. 209°; this boiled 4 hrs. with HOAc-HCl gave 2-phenylcoumarone (VI), which was hydrolyzed by refluxing 10 min. with 10% alc. NaOH, to give a mixture of unchanged material, VI, and 3-benzoylisocoumaranone (VII), m. 100°. Ultraviolet absorption spectrum of VII showed  $\lambda$  232, 252, and 339 m $\mu$ ,  $\epsilon$  11,589, 13,169, and 11,026 in alc. and infrared spectrum (KBr pellet, 1% weight/weight)  $\lambda$  5.93, 6.15, 6.70, 6.91, 7.45, 8.03, 8.24, 8.48, 8.58 and 8.68. IV and 3-o-hydroxyphenylacetylisocoumaranone phenylhydrazone yielded 4-o-hydroxyphenyl-3-methyl (and 3-o-hydroxytolyl)-1-phenylpyrazol-5-one, m. 201-2° and 224°, resp. (both from EtOH), on boiling with alc. 10% HCl 2-3 hrs. VII gave the corresponding pyrazolone, m. 145° (EtOH) in crude form merely by keeping it 12 days in cold with PhNHNH<sub>2</sub> in alc. The acylation of I by heating with acid chlorides in C<sub>5</sub>H<sub>5</sub>N gave polymethines of the type o-C<sub>6</sub>H<sub>4</sub>.O.CO.C:CRNCHCH:CHCH:CHC:C(OH).O.C<sub>6</sub>H<sub>4</sub>-o (VIII) (Pfeiffer and Enders, C.A. 45, 9047e), characterized by the color changes from red or brownish red to blue or green, and a yellow by-product, m. 305°, identified as 3,4,7,8-dibenzonaphthyrone (IX). The following polymethines were also prepared (R and m.p. given): p-tolyl, 268-9° (decomposition); p-anisyl, 255° (decomposition), and m-chlorophenyl, 260° (decomposition). Polymethines were also obtained by condensation of Zincke aldehyde (loc. cit.) with the reactive methylene groups in coumaranone, thioindoxyl, and 1,3-dioxohydrindene to give condensation compds., m. 232°, 266° (decomposition), and 275° (decomposition), resp. The structure of IX was confirmed by synthesis of isooxindigo (X) (Chovin, C.A. 37, 2737i) and its isomerization to IX by heating 15 hrs. with C<sub>5</sub>H<sub>5</sub>N at 100°. I (1.5 g.) heated 18 hrs. at 100° with C<sub>5</sub>H<sub>5</sub>N only, cooled, 2 cc. alc. added and refrigerated 1 week gave IX, yellow needles

(HOAc), thus accounting for its presence in these reactions. Ultraviolet and infrared data were given for IX and I and compared with those for X. IX absorbed a mole of H (PtO<sub>2</sub>-HOAc) to give a mixture of colorless, stereoisomerides from which 1 component was isolated as plates, m. 218° (HOAc). Thiooxindole gave only intractable tar with warm C<sub>5</sub>H<sub>5</sub>N. Coumaranone (1.0 g.) heated, 48 hrs., with 5 cc. C<sub>5</sub>H<sub>5</sub>N gave only 10 mg. of s-tris-coumaronobenzene, m. above 360° (xylene) (cf. C.A. 33, 33631). 1,3-Dioxohydrindene (0.5 g.) heated, 0.5 hr., with 2 cc. C<sub>5</sub>H<sub>5</sub>N gave 20 mg. trisbenzoylenebenzene, m. above 360°.

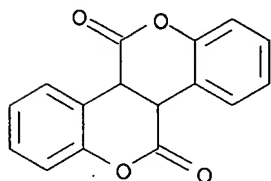
IT **13225-81-5**, Fumaric acid, bis(o-hydroxyphenyl)-, di-8-lactone  
(preparation of)  
RN 13225-81-5 CAPLUS  
CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione (8CI, 9CI) (CA INDEX NAME)



IT **20752-64-1**, [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 4b,10b-dihydro- **101279-18-9**, Succinic acid, 2,3-bis(o-hydroxyphenyl)-, di-8-lactone  
(stereoisomers)  
RN 20752-64-1 CAPLUS  
CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione, 4b,10b-dihydro- (8CI) (CA INDEX NAME)



RN 101279-18-9 CAPLUS  
CN Succinic acid, 2,3-bis(o-hydroxyphenyl)-, di-8-lactone (6CI) (CA INDEX NAME)



1022 ANSWER 56 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1945:5964 CAPLUS

DOCUMENT NUMBER: 39:5964

ORIGINAL REFERENCE NO.: 39:932c-h

TITLE: Colored lactones. Isooxindigo and benzonaphthyrones

AUTHOR(S): Chovin, P.

SOURCE: Bull. soc. chim. (1944), 11, 82-90

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

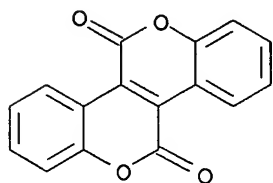
AB cf. C. A. 37, 2737.1. o-HOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CO<sub>2</sub>H (I) and BzCH<sub>2</sub>COCO<sub>2</sub>H (II) heated at 125° for 20 min. in the presence of PBr<sub>3</sub> give 22% of a red compound (III), m. 269.5°, which is either IV or V (R = Ph). A 5% yield of III is obtained from o-HOC<sub>6</sub>H<sub>4</sub>COCO<sub>2</sub>H (VI) and BzCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H under the same conditions. A similar red compound (R = C<sub>6</sub>H<sub>4</sub>Br) (VII) is obtained in 22-5% yield from VI and BrC<sub>6</sub>H<sub>4</sub>COCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H. When I and VI are heated with PBr<sub>3</sub> they give 32-6% of an orange compound (VIII), m. 283°, which is either isooxindigo (IX) or 3,4,7,8-dibenzonaphthyrone (X). α-Coumaranone (XI) and coumarandione (XII) in AcOH in the presence of H<sub>2</sub>SO<sub>4</sub> give in the cold 3-5% VIII. When heated with PBr<sub>3</sub>, XI and XII give 50-8% VIII. Heating XI with SOCl<sub>2</sub> gives 15-20% VIII, and with S<sub>2</sub>Cl<sub>2</sub>, 30-50%. Since β-coumaranone and S<sub>2</sub>Cl<sub>2</sub> give 50% oxindigo, oxindol and S<sub>2</sub>Cl<sub>2</sub> give 90% isoindigo and 3-hydroxythianaphthene and S<sub>2</sub>Cl<sub>2</sub> give 75% thioindigo, the reaction is general. Ozonolysis of VIII gives an ozonide which decomps. in AcOH to XII and salicylic acid. When VIII is heated with 10% alc. KOH it gives 100% of a yellow isomer (XIII). VIII and HCONH<sub>2</sub> (XIV) give 60% XIII, m. 305°. XIII gives an ozonide m. 269° which decomps. to XII when heated. When the Pechmann dye is heated with XIV it gives 75% of a brownish green, insol. compound m. above 500°. Under these conditions, III gives a yellow-brown compound m. 305°, and VII a similar compound m. 339°. XI and Me<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>NO give 37%. coumarandione p-dimethylaminoanil, m. 245°. These reactions indicate, but do not prove, that VIII is IX and XIII is X.

IT 13225-81-5, Fumaric acid, bis(o-hydroxyphenyl)-, di-8-lactone

(preparation of)

RN 13225-81-5 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione (8CI, 9CI) (CA INDEX NAME)



L22 ANSWER 57 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1945:1799 CAPLUS

DOCUMENT NUMBER: 39:1799

ORIGINAL REFERENCE NO.: 39:297h-i,298a

TITLE: Isooxindigo

AUTHOR(S): Chovin, Paul

SOURCE: Compt. rend. (1942), 215, 466-8

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

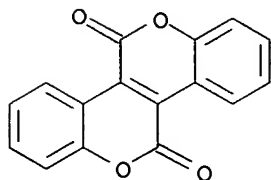
AB cf. C. A. 37, 2737.1. In condensing o-HOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CO<sub>2</sub>H with o-HOC<sub>6</sub>H<sub>4</sub>COCO<sub>2</sub>H by using PBr<sub>3</sub>, an orange compound (I) is formed (35%) which possesses 2 lactonic functions, and the di-K salt of which, when treated with HCl, gives a yellow compound (II). Whether I or II is isooxindigo is not proven, and color analogy with other members of the indigo series is not certain proof. Indications that I is isooxindigo and II is dibenzonaphthyrone are (a) α-coumaronone with S<sub>2</sub>Cl<sub>2</sub> gives I exclusively, in 50% yield. By analogy then isooxindigo is I. (b) When the lactones of o-HOC<sub>6</sub>H<sub>4</sub>COCO<sub>2</sub>H acid and o-HOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CO<sub>2</sub>H are used, I is formed in 50-60% yield. Ozonization of I and II was not decisive to decide which compound was isooxindigo and which compound was dibenzonaphthyrone.

IT 13225-81-5, Fumaric acid, bis(o-hydroxyphenyl)-, di-8-lactone

(preparation of)

RN 13225-81-5 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione (8CI, 9CI) (CA INDEX NAME)



~~L22~~ ANSWER 58 OF 58 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1943:16719 CAPLUS

DOCUMENT NUMBER: 37:16719

ORIGINAL REFERENCE NO.: 37:2737a-e

TITLE: Colored lactones. 3,4,7,8-Dibenzonaphthyrone, an isomer of oxindigo

AUTHOR(S): Chovin, Paul

SOURCE: Compt. rend. (1941), 212, 549-51

From: Chem. Zentr. 1942, I, 614.

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

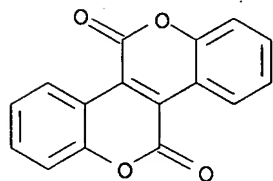
AB cf. C. A. 36, 2258.5. In analogy with the preparation of the red-violet 3,7-diphenylnaphthyrone and the red-orange 3-phenyl-7,8-benzonaphthyrone, the yellow-orange 3,4,7,8-dibenzonaphthyrone, C<sub>16</sub>H<sub>8</sub>O<sub>4</sub> (I), m. 283°, is obtained by condensation of o-HOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CO<sub>2</sub>H and o-HOC<sub>6</sub>H<sub>4</sub>COCO<sub>2</sub>H. I is an isomer of oxindigo. In addition there exists a closer relationship between naphthyrones and oxindigo, since under certain conditions there are formed in the preparation of diarylnaphthyrones yellow isomers (II) as by-products; the isomer corresponding to I would be the still unknown isooxindigo (III). However, fractional crystallization and chromatographic analysis gave no indications that III was present besides I in the crude reaction product. The synthesis of III may, however, be possible under different exptl. conditions.

IT 13225-81-5, Fumaric acid, bis(o-hydroxyphenyl)-, di-8-lactone

(preparation of)

RN 13225-81-5 CAPLUS

CN [1]Benzopyrano[4,3-c][1]benzopyran-5,11-dione (8CI, 9CI) (CA INDEX NAME)





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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

292.46

692.21

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

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